

# Supporting Information: A Fixed-charge Model for Alcohol Polarization in the Condensed-phase, and its Role in Small Molecule Hydration

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## Supporting Information Overview

This document contains results for the  $\epsilon(0)$  calculations on 41 neat liquids, the results for the transfer free energy calculations discussed in the text, coordinates and charges for all the solutes, and the source code for perl and python scripts that apply the DC modifications to hydroxyl groups in GROMACS topology files. Future updates of these programs can be found on the author research group websites.

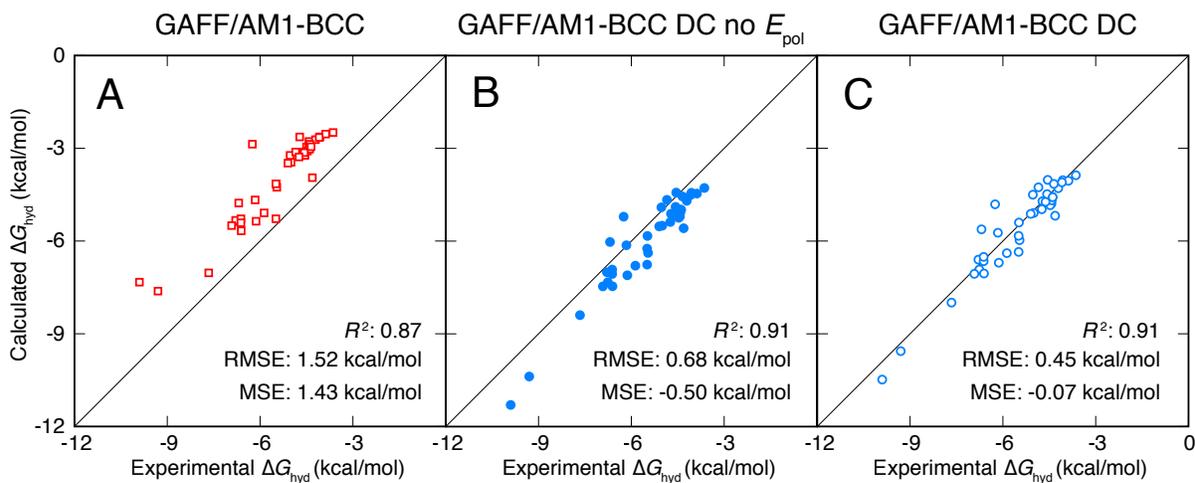


Figure SI 1: Scatterplots and statistical analysis of the hydration data listed in Table SI 2. Sub-plots A, B, and C are GAFF/AM1-BCC, GAFF/AM1-BCC DC w/o  $E_{pol}$ , and GAFF/AM1-BCC DC respectively. Without the 0.409 kcal/mol per-hydroxyl  $E_{pol}$  term, the DC parameters tend to lead to a slight over-solvation of hydroxyl groups, but the RMSE and MSE metrics are both near 1  $kT$ . Inclusion of the  $E_{pol}$  term improves all the performance metrics in the calculation of  $\Delta G_{hyd}$ .

Table SI 1: Experimental versus calculated  $\epsilon(0)$  using GAFF/AM1-BCC and GAFF/AM1-BCC DC

Name	Expt.	T (K)	GAFF/AM1-BCC	GAFF/AM1-BCC DC
12_ethanediol	40.6	298.15	25.4 $\pm$ 0.2	35.4 $\pm$ 0.3
13_propanediol	34.3	298.15	21.4 $\pm$ 0.2	37.2 $\pm$ 0.9
2_butoxyethanol	9.4	298.15	5.63 $\pm$ 0.03	7.0 $\pm$ 0.1
2_chlorophenol	7.2	298.15	3.385 $\pm$ 0.009	2.91 $\pm$ 0.02
2_ethoxyethanol	13.4	298.15	8.98 $\pm$ 0.06	11.4 $\pm$ 0.2
2_methoxyethanol	17.2	298.15	17.09 $\pm$ 0.08	21.6 $\pm$ 0.3
2_methylbutan_1_ol	15.4	298.15	7.23 $\pm$ 0.09	13 $\pm$ 1
2_methylbutan_2_ol	5.8	298.15	4.77 $\pm$ 0.02	7.3 $\pm$ 0.7
2_methylpropan_1_ol	17.2	298.15	8.36 $\pm$ 0.06	14.5 $\pm$ 0.6
2_methylpropan_2_ol	12	298.15	8.3 $\pm$ 0.1	7.5 $\pm$ 0.9
2_phenylethanol	11.9	298.15	5.82 $\pm$ 0.03	10.0 $\pm$ 0.7
222_trifluoroethanol	26.8	298.15	19.10 $\pm$ 0.03	26.5 $\pm$ 0.4
23_dimethylphenol	4.8	343.15	2.519 $\pm$ 0.008	3.81 $\pm$ 0.02
3_chlorophenol	6.3	293.15	5.51 $\pm$ 0.04	6.96 $\pm$ 0.08
3_methoxyphenol	11.6	298.15	7.07 $\pm$ 0.03	9.8 $\pm$ 0.5
3_methylbutan_1_ol	14.8	298.15	8.1 $\pm$ 0.1	13.8 $\pm$ 0.5
3_phenylpropanol	11.6	298.15	5.29 $\pm$ 0.04	8.1 $\pm$ 0.9
benzyl_alcohol	12.2	303.15	6.81 $\pm$ 0.08	11.0 $\pm$ 0.2
butan_1_ol	17.5	298.15	9.39 $\pm$ 0.09	16.1 $\pm$ 0.3
butan_2_ol	16.7	298.15	9.0 $\pm$ 0.2	12.9 $\pm$ 0.4
cycloheptanol	13.5	293.15	8.5 $\pm$ 0.2	3.4 $\pm$ 0.4
cyclohexanol	16.1	298.15	8.9 $\pm$ 0.4	5.8 $\pm$ 0.6
cyclopentanol	17.5	298.15	9.3 $\pm$ 0.1	13.6 $\pm$ 0.4
decan_1_ol	7.62	298.15	3.8 $\pm$ 0.1	3.4 $\pm$ 0.2
ethanol	24.8	298.15	14.0 $\pm$ 0.1	24.0 $\pm$ 0.4
heptan_1_ol	11.5	298.15	5.98 $\pm$ 0.09	8.9 $\pm$ 0.4
hexan_1_ol	12.5	298.15	6.9 $\pm$ 0.1	10.6 $\pm$ 0.6
hexan_3_ol	9.7	298.15	6.04 $\pm$ 0.09	3.9 $\pm$ 0.5
m_cresol	12.4	298.15	3.91 $\pm$ 0.01	5.65 $\pm$ 0.05
methanol	31.9	298.15	20.13 $\pm$ 0.05	34.1 $\pm$ 0.2
nonan_1_ol	8.6	298.15	4.7 $\pm$ 0.2	6.2 $\pm$ 0.2
o_cresol	6.8	298.15	3.214 $\pm$ 0.004	4.96 $\pm$ 0.07
octan_1_ol	9.7	298.15	5.2 $\pm$ 0.1	6.8 $\pm$ 0.7
p_cresol	12.6	298.15	5.66 $\pm$ 0.08	8.1 $\pm$ 0.1
pentan_1_ol	14.6	298.15	7.9 $\pm$ 0.1	14.5 $\pm$ 0.9
pentan_2_ol	12.8	298.15	7.49 $\pm$ 0.07	11 $\pm$ 1
pentan_3_ol	12.8	298.15	7.5 $\pm$ 0.1	7.3 $\pm$ 0.3
phenol	11.1	318.15	6.14 $\pm$ 0.06	11.1 $\pm$ 0.1
prop_2_en_1_ol	18.9	298.15	11.4 $\pm$ 0.1	19.4 $\pm$ 0.2
propan_1_ol	20.3	298.15	10.88 $\pm$ 0.05	18.9 $\pm$ 0.2
propan_2_ol	19.1	298.15	11.5 $\pm$ 0.1	20.0 $\pm$ 0.9

Table SI 2: Experimental versus calculated  $\Delta G_{\text{hyd}}$  in kcal/mol using the original and modified forms of GAFF with AM1-BCC partial charges

Name	Expt.	GAFF/AM1-BCC	GAFF/AM1-BCC DC w/o $E_{\text{pol}}$	GAFF/AM1-BCC DC
12_ethanediol	-9.3	-7.62 $\pm$ 0.03	-10.38 $\pm$ 0.02	-9.56 $\pm$ 0.02
13_propanediol	-9.9	-7.33 $\pm$ 0.02	-11.30 $\pm$ 0.03	-10.48 $\pm$ 0.03
2_butoxyethanol	-6.25	-2.87 $\pm$ 0.03	-5.21 $\pm$ 0.03	-4.81 $\pm$ 0.03
2_chlorophenol	-4.55	-3.23 $\pm$ 0.03	-4.43 $\pm$ 0.08	-4.02 $\pm$ 0.08
2_ethoxyethanol	-6.69	-4.77 $\pm$ 0.03	-6.03 $\pm$ 0.03	-5.62 $\pm$ 0.03
2_methoxyethanol	-6.76	-5.37 $\pm$ 0.03	-7.33 $\pm$ 0.02	-6.92 $\pm$ 0.02
2_methylbutan_1_ol	-4.42	-2.78 $\pm$ 0.02	-5.01 $\pm$ 0.02	-4.60 $\pm$ 0.02
2_methylbutan_2_ol	-4.43	-2.96 $\pm$ 0.03	-5.20 $\pm$ 0.02	-4.79 $\pm$ 0.02
2_methylpropan_1_ol	-4.5	-2.96 $\pm$ 0.02	-5.05 $\pm$ 0.02	-4.64 $\pm$ 0.02
2_methylpropan_2_ol	-4.47	-3.09 $\pm$ 0.02	-5.25 $\pm$ 0.02	-4.84 $\pm$ 0.02
2_phenylethanol	-6.79	-5.33 $\pm$ 0.03	-7.01 $\pm$ 0.03	-6.60 $\pm$ 0.03
222_trifluoroethanol	-4.31	-3.95 $\pm$ 0.03	-5.58 $\pm$ 0.02	-5.18 $\pm$ 0.02
23_dimethylphenol	-6.16	-4.67 $\pm$ 0.03	-6.13 $\pm$ 0.02	-5.73 $\pm$ 0.02
3_chlorophenol	-6.62	-5.28 $\pm$ 0.03	-7.06 $\pm$ 0.02	-6.65 $\pm$ 0.02
3_methoxyphenol	-7.66	-7.03 $\pm$ 0.03	-8.40 $\pm$ 0.03	-7.99 $\pm$ 0.03
3_methylbutan_1_ol	-4.42	-2.92 $\pm$ 0.03	-5.09 $\pm$ 0.03	-4.68 $\pm$ 0.03
3_phenylpropanol	-6.92	-5.50 $\pm$ 0.03	-7.46 $\pm$ 0.03	-7.06 $\pm$ 0.03
benzyl_alcohol	-6.62	-5.41 $\pm$ 0.03	-6.92 $\pm$ 0.02	-6.51 $\pm$ 0.02
butan_1_ol	-4.72	-2.63 $\pm$ 0.02	-5.12 $\pm$ 0.02	-4.71 $\pm$ 0.02
butan_2_ol	-4.62	-3.12 $\pm$ 0.03	-5.14 $\pm$ 0.02	-4.73 $\pm$ 0.02
cycloheptanol	-5.48	-4.15 $\pm$ 0.05	-5.8 $\pm$ 0.2	-5.4 $\pm$ 0.2
cyclohexanol	-5.46	-4.26 $\pm$ 0.02	-6.38 $\pm$ 0.02	-5.97 $\pm$ 0.02
cyclopentanol	-5.49	-4.15 $\pm$ 0.02	-6.24 $\pm$ 0.02	-5.83 $\pm$ 0.02
decan_1_ol	-3.64	-2.49 $\pm$ 0.03	-4.28 $\pm$ 0.06	-3.87 $\pm$ 0.06
ethanol	-5	-3.45 $\pm$ 0.03	-5.50 $\pm$ 0.02	-5.09 $\pm$ 0.02
heptan_1_ol	-4.21	-2.72 $\pm$ 0.02	-4.70 $\pm$ 0.04	-4.29 $\pm$ 0.04
hexan_1_ol	-4.4	-3.03 $\pm$ 0.02	-4.98 $\pm$ 0.03	-4.57 $\pm$ 0.03
hexan_3_ol	-4.06	-2.63 $\pm$ 0.02	-4.44 $\pm$ 0.04	-4.03 $\pm$ 0.04
m_cresol	-5.49	-5.28 $\pm$ 0.03	-6.76 $\pm$ 0.02	-6.35 $\pm$ 0.02
methanol	-5.1	-3.48 $\pm$ 0.01	-5.52 $\pm$ 0.01	-5.12 $\pm$ 0.01
nonan_1_ol	-3.88	-2.54 $\pm$ 0.03	-4.46 $\pm$ 0.05	-4.05 $\pm$ 0.05
o_cresol	-5.87	-5.09 $\pm$ 0.02	-6.80 $\pm$ 0.02	-6.39 $\pm$ 0.02
octan_1_ol	-4.09	-2.65 $\pm$ 0.03	-4.51 $\pm$ 0.04	-4.10 $\pm$ 0.04
p_cresol	-6.13	-5.36 $\pm$ 0.02	-7.11 $\pm$ 0.02	-6.70 $\pm$ 0.02
pentan_1_ol	-4.57	-3.14 $\pm$ 0.02	-4.89 $\pm$ 0.03	-4.48 $\pm$ 0.03
pentan_2_ol	-4.39	-2.87 $\pm$ 0.02	-4.99 $\pm$ 0.03	-4.58 $\pm$ 0.03
pentan_3_ol	-4.35	-2.95 $\pm$ 0.02	-4.55 $\pm$ 0.03	-4.15 $\pm$ 0.03
phenol	-6.61	-5.67 $\pm$ 0.03	-7.46 $\pm$ 0.02	-7.05 $\pm$ 0.02
prop_2_en_1_ol	-5.03	-3.23 $\pm$ 0.03	-4.91 $\pm$ 0.02	-4.50 $\pm$ 0.02
propan_1_ol	-4.85	-3.12 $\pm$ 0.02	-4.66 $\pm$ 0.02	-4.26 $\pm$ 0.02
propan_2_ol	-4.74	-3.28 $\pm$ 0.02	-5.38 $\pm$ 0.02	-4.97 $\pm$ 0.02

Table SI 3: Experimental versus calculated  $\Delta G_{\text{hyd}}$  in kcal/mol using the original and modified forms of GAFF with AM1-BCC partial charges for the SAMPL4 solutes containing hydroxyl groups

Name	Expt.	GAFF/AM1-BCC	GAFF/AM1-BCC DC w/o $E_{\text{pol}}$	GAFF/AM1-BCC DC
SAMPL4_001	-23.6	-18.64 $\pm$ 0.04	-22.34 $\pm$ 0.05	-19.89 $\pm$ 0.05
SAMPL4_003	-4.8	-2.64 $\pm$ 0.02	-4.22 $\pm$ 0.02	-3.81 $\pm$ 0.02
SAMPL4_004	-4.5	-2.54 $\pm$ 0.02	-4.22 $\pm$ 0.02	-3.81 $\pm$ 0.02
SAMPL4_006	-5.3	-4.10 $\pm$ 0.02	-5.23 $\pm$ 0.02	-4.82 $\pm$ 0.02
SAMPL4_009	-8.2	-9.94 $\pm$ 0.02	-11.38 $\pm$ 0.03	-10.97 $\pm$ 0.03
SAMPL4_010	-6.2	-6.13 $\pm$ 0.02	-7.55 $\pm$ 0.02	-7.14 $\pm$ 0.02
SAMPL4_011	-7.8	-9.23 $\pm$ 0.03	-10.57 $\pm$ 0.03	-10.57 $\pm$ 0.03
SAMPL4_013	-4.4	-3.38 $\pm$ 0.02	-5.05 $\pm$ 0.02	-4.64 $\pm$ 0.02
SAMPL4_016	-3.2	-3.39 $\pm$ 0.02	-5.26 $\pm$ 0.02	-4.85 $\pm$ 0.02
SAMPL4_025	-5.7	-3.78 $\pm$ 0.02	-5.16 $\pm$ 0.02	-4.75 $\pm$ 0.02
SAMPL4_032	-7.3	-5.32 $\pm$ 0.02	-6.89 $\pm$ 0.02	-6.48 $\pm$ 0.02
SAMPL4_033	-7	-7.05 $\pm$ 0.02	-8.91 $\pm$ 0.02	-8.50 $\pm$ 0.02
SAMPL4_034	-5.8	-4.46 $\pm$ 0.02	-5.62 $\pm$ 0.02	-5.21 $\pm$ 0.02
SAMPL4_035	-4.7	-4.89 $\pm$ 0.02	-5.03 $\pm$ 0.02	-4.62 $\pm$ 0.02
SAMPL4_036	-5.7	-4.70 $\pm$ 0.02	-6.28 $\pm$ 0.02	-5.87 $\pm$ 0.02
SAMPL4_037	-5.9	-4.62 $\pm$ 0.02	-5.84 $\pm$ 0.02	-5.43 $\pm$ 0.02
SAMPL4_047	-14.2	-13.33 $\pm$ 0.03	-14.67 $\pm$ 0.03	-14.26 $\pm$ 0.03
SAMPL4_051	-9.5	-11.22 $\pm$ 0.02	-11.33 $\pm$ 0.02	-10.92 $\pm$ 0.02

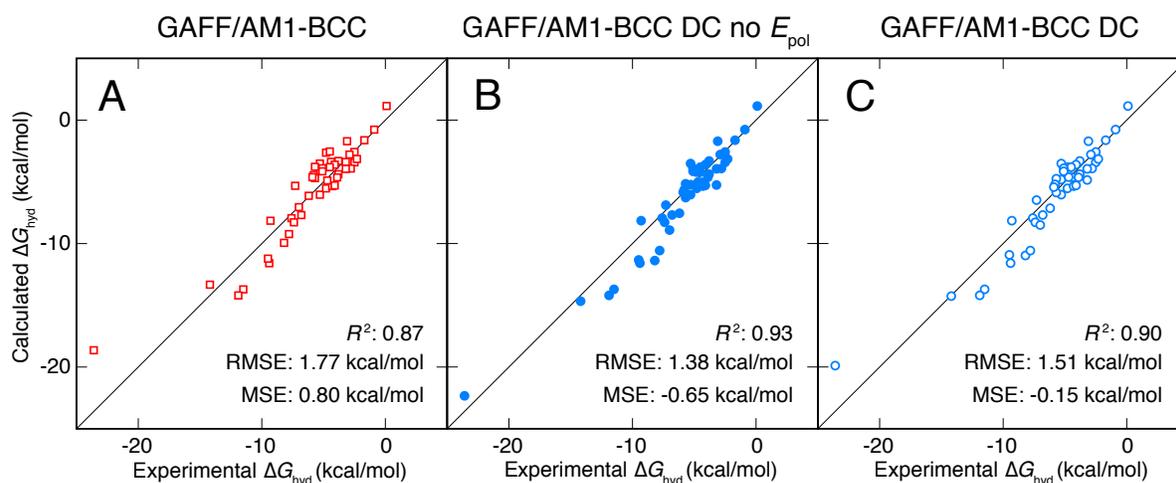


Figure SI 2: Scatterplots and statistical analysis of the hydration data listed in Table SI 3. Plotted are both the SAMPL4 solutes that contain hydroxyl groups (Table SI 3) and non-hydroxyl containing solutes (data available from the SAMPL4 publications cited in the main text). As labeled plots A, B, and C are GAFF/AM1-BCC, GAFF/AM1-BCC DC w/o  $E_{\text{pol}}$ , and GAFF/AM1-BCC DC respectively. Without the 0.409 kcal/mol per-hydroxyl  $E_{\text{pol}}$  term, the DC parameters improve upon the results for unmodified solutes in all listed metrics. Inclusion of the  $E_{\text{pol}}$  term improves the MSE, but there is a slight degradation of the  $\Delta G_{\text{hyd}}$  RMSE, almost entirely due to shift of a single molecule (mannitol) with a very favorable solvation energy.

## GROMACS configuration files for molecules used in this study.

12\_ethanediol

10

1TMP	C1	1	3.817	3.795	1.762
1TMP	C2	2	3.691	3.731	1.706
1TMP	O1	3	3.821	3.774	1.903
1TMP	O2	4	3.695	3.591	1.732
1TMP	H1	5	3.817	3.903	1.744
1TMP	H2	6	3.906	3.750	1.718
1TMP	H3	7	3.685	3.745	1.598
1TMP	H4	8	3.602	3.772	1.754
1TMP	H5	9	3.816	3.861	1.944
1TMP	H6	10	3.646	3.576	1.814

5.00000 5.00000 3.53553 0.00000 0.00000 0.00000 0.00000 2.50000 2.50000

13\_propanediol

13

1	UNK	O1	1	9.381	5.770	2.187
1	UNK	C1	2	9.522	5.756	2.204
1	UNK	C2	3	9.557	5.606	2.212
1	UNK	C3	4	9.708	5.587	2.230
1	UNK	O2	5	9.736	5.447	2.238
1	UNK	H12	6	9.553	5.806	2.296
1	UNK	H13	7	9.573	5.801	2.119
1	UNK	H22	8	9.503	5.561	2.296
1	UNK	H23	9	9.524	5.556	2.121
1	UNK	H32	10	9.762	5.630	2.146
1	UNK	H33	11	9.741	5.635	2.323
1	UNK	HO2	12	9.832	5.434	2.249
1	UNK	HO1	13	9.359	5.864	2.182

5.00000 5.00000 3.53553 0.00000 0.00000 0.00000 0.00000 2.50000 2.50000

2\_butoxyethanol

22

1TMP	C1	1	4.085	3.911	1.763
1TMP	C2	2	3.987	3.813	1.826
1TMP	C3	3	3.851	3.818	1.756
1TMP	C4	4	3.754	3.717	1.816
1TMP	C5	5	3.405	3.649	1.721
1TMP	C6	6	3.535	3.634	1.798
1TMP	O1	7	3.430	3.623	1.583
1TMP	O2	8	3.630	3.725	1.746
1TMP	H1	9	4.101	3.887	1.657
1TMP	H2	10	4.048	4.014	1.769
1TMP	H3	11	4.181	3.906	1.814
1TMP	H4	12	4.028	3.712	1.821
1TMP	H5	13	3.975	3.838	1.932
1TMP	H6	14	3.808	3.918	1.763
1TMP	H7	15	3.863	3.797	1.649
1TMP	H8	16	3.792	3.615	1.808
1TMP	H9	17	3.735	3.740	1.922
1TMP	H10	18	3.365	3.750	1.730
1TMP	H11	19	3.331	3.577	1.757
1TMP	H12	20	3.575	3.533	1.788
1TMP	H13	21	3.519	3.657	1.904
1TMP	H14	22	3.511	3.670	1.560

5.00000 5.00000 3.53553 0.00000 0.00000 0.00000 0.00000 2.50000 2.50000

2\_chlorophenol

13

1TMP	C1	1	2.036	2.505	1.255
1TMP	C2	2	2.146	2.543	1.328
1TMP	C3	3	2.002	2.371	1.228
1TMP	C4	4	2.226	2.438	1.387
1TMP	C5	5	2.084	2.274	1.278
1TMP	C6	6	2.191	2.304	1.360
1TMP	O1	7	2.061	2.148	1.226
1TMP	C11	8	2.293	2.186	1.430
1TMP	H1	9	1.973	2.578	1.204
1TMP	H2	10	2.175	2.643	1.358
1TMP	H3	11	1.930	2.350	1.150
1TMP	H4	12	2.306	2.462	1.457

1TMP	H5	13	2.004	2.086	1.275					
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000	
2_ethoxyethanol										
16										
1TMP	C1	1	3.493	3.793	1.792					
1TMP	C2	2	3.610	3.710	1.742					
1TMP	C3	3	3.970	3.756	1.806					
1TMP	C4	4	3.844	3.692	1.750					
1TMP	O1	5	3.979	3.890	1.758					
1TMP	O2	6	3.731	3.765	1.794					
1TMP	H1	7	3.399	3.753	1.754					
1TMP	H2	8	3.490	3.793	1.901					
1TMP	H3	9	3.503	3.897	1.760					
1TMP	H4	10	3.615	3.712	1.633					
1TMP	H5	11	3.601	3.607	1.776					
1TMP	H6	12	4.059	3.702	1.775					
1TMP	H7	13	3.965	3.759	1.915					
1TMP	H8	14	3.834	3.588	1.785					
1TMP	H9	15	3.846	3.693	1.641					
1TMP	H10	16	4.060	3.894	1.704					
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000	
2_methoxyethanol										
13										
1TMP	C1	1	3.542	3.724	1.745					
1TMP	C2	2	3.902	3.770	1.809					
1TMP	C3	3	3.776	3.706	1.753					
1TMP	O1	4	3.911	3.904	1.761					
1TMP	O2	5	3.663	3.779	1.797					
1TMP	H1	6	3.457	3.783	1.781					
1TMP	H2	7	3.532	3.621	1.778					
1TMP	H3	8	3.546	3.728	1.636					
1TMP	H4	9	3.991	3.716	1.778					
1TMP	H5	10	3.897	3.773	1.918					
1TMP	H6	11	3.766	3.602	1.788					
1TMP	H7	12	3.778	3.707	1.644					
1TMP	H8	13	3.992	3.941	1.799					
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000	
2_methylbutan_1_ol										
18										
1TMP	C1	1	3.763	3.929	1.880					
1TMP	C2	2	3.845	3.774	1.639					
1TMP	C3	3	3.748	3.778	1.870					
1TMP	C4	4	3.714	3.574	1.718					
1TMP	C5	5	3.728	3.727	1.726					
1TMP	O1	6	3.605	3.530	1.797					
1TMP	H1	7	3.855	3.964	1.833					
1TMP	H2	8	3.678	3.980	1.832					
1TMP	H3	9	3.764	3.960	1.985					
1TMP	H4	10	3.941	3.731	1.673					
1TMP	H5	11	3.855	3.883	1.642					
1TMP	H6	12	3.830	3.745	1.535					
1TMP	H7	13	3.662	3.748	1.931					
1TMP	H8	14	3.836	3.731	1.916					
1TMP	H9	15	3.805	3.524	1.752					
1TMP	H10	16	3.695	3.544	1.614					
1TMP	H11	17	3.636	3.772	1.686					
1TMP	H12	18	3.539	3.602	1.799					
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000	
2_methylbutan_2_ol										
18										
1TMP	C1	1	3.926	3.753	1.889					
1TMP	C2	2	3.774	3.675	1.632					
1TMP	C3	3	3.583	3.814	1.714					
1TMP	C4	4	3.802	3.823	1.837					
1TMP	C5	5	3.707	3.734	1.756					
1TMP	O1	6	3.663	3.625	1.837					
1TMP	H1	7	3.985	3.821	1.952					
1TMP	H2	8	3.991	3.720	1.807					
1TMP	H3	9	3.900	3.665	1.950					
1TMP	H4	10	3.815	3.753	1.567					
1TMP	H5	11	3.855	3.605	1.659					
1TMP	H6	12	3.703	3.615	1.573					

1TMP	H7	13	3.609	3.898	1.648				
1TMP	H8	14	3.511	3.750	1.661				
1TMP	H9	15	3.530	3.853	1.802				
1TMP	H10	16	3.833	3.910	1.777				
1TMP	H11	17	3.748	3.863	1.924				
1TMP	H12	18	3.567	3.622	1.829				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
2_methylpropan_1_ol									
15									
1TMP	C1	1	3.691	3.616	1.811				
1TMP	C2	2	3.707	3.770	1.613				
1TMP	C3	3	3.791	3.847	1.837				
1TMP	C4	4	3.773	3.727	1.744				
1TMP	O1	5	3.860	3.807	1.954				
1TMP	H1	6	3.679	3.531	1.743				
1TMP	H2	7	3.591	3.652	1.838				
1TMP	H3	8	3.740	3.580	1.901				
1TMP	H4	9	3.696	3.685	1.545				
1TMP	H5	10	3.767	3.846	1.562				
1TMP	H6	11	3.607	3.812	1.631				
1TMP	H7	12	3.850	3.925	1.787				
1TMP	H8	13	3.694	3.889	1.866				
1TMP	H9	14	3.872	3.685	1.721				
1TMP	H10	15	3.932	3.871	1.967				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
2_methylpropan_2_ol									
15									
1TMP	C1	1	3.638	3.776	1.682				
1TMP	C2	2	3.848	3.852	1.799				
1TMP	C3	3	3.805	3.607	1.764				
1TMP	C4	4	3.741	3.743	1.790				
1TMP	O1	5	3.674	3.738	1.916				
1TMP	H1	6	3.589	3.872	1.703				
1TMP	H2	7	3.685	3.783	1.583				
1TMP	H3	8	3.559	3.701	1.678				
1TMP	H4	9	3.919	3.831	1.879				
1TMP	H5	10	3.803	3.949	1.822				
1TMP	H6	11	3.904	3.861	1.705				
1TMP	H7	12	3.730	3.528	1.762				
1TMP	H8	13	3.860	3.606	1.669				
1TMP	H9	14	3.875	3.581	1.845				
1TMP	H10	15	3.619	3.818	1.921				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
2_phenylethanol									
19									
1TMP	C1	1	3.736	3.717	1.488				
1TMP	C2	2	3.629	3.777	1.555				
1TMP	C3	3	3.841	3.661	1.560				
1TMP	C4	4	3.627	3.780	1.695				
1TMP	C5	5	3.839	3.664	1.700				
1TMP	C6	6	3.732	3.723	1.767				
1TMP	C7	7	3.730	3.727	1.916				
1TMP	C8	8	3.798	3.851	1.974				
1TMP	O1	9	3.789	3.849	2.116				
1TMP	H1	10	3.737	3.715	1.379				
1TMP	H2	11	3.547	3.821	1.499				
1TMP	H3	12	3.924	3.614	1.508				
1TMP	H4	13	3.543	3.827	1.746				
1TMP	H5	14	3.921	3.619	1.755				
1TMP	H6	15	3.780	3.637	1.957				
1TMP	H7	16	3.626	3.722	1.952				
1TMP	H8	17	3.746	3.942	1.939				
1TMP	H9	18	3.903	3.857	1.945				
1TMP	H10	19	3.794	3.756	2.142				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
222_trifluoroethanol									
9									
1TMP	C1	1	3.707	3.714	1.738				
1TMP	C2	2	3.764	3.831	1.813				
1TMP	O1	3	3.811	3.651	1.665				
1TMP	F1	4	3.861	3.791	1.899				
1TMP	F2	5	3.669	3.894	1.886				

1TMP	F3	6	3.819	3.922	1.729				
1TMP	H1	7	3.664	3.641	1.807				
1TMP	H2	8	3.630	3.747	1.668				
1TMP	H3	9	3.823	3.562	1.703				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
23_dimethylphenol									
19									
1TMP	C1	1	2.359	2.718	0.784				
1TMP	C2	2	2.469	2.690	0.865				
1TMP	C3	3	2.253	2.629	0.775				
1TMP	C4	4	2.473	2.571	0.938				
1TMP	C5	5	2.363	2.483	0.919				
1TMP	C6	6	2.261	2.508	0.834				
1TMP	C7	7	2.574	2.566	1.047				
1TMP	C8	8	2.370	2.350	0.992				
1TMP	O1	9	2.167	2.413	0.819				
1TMP	H1	10	2.348	2.812	0.731				
1TMP	H2	11	2.544	2.767	0.881				
1TMP	H3	12	2.177	2.653	0.701				
1TMP	H4	13	2.671	2.607	1.018				
1TMP	H5	14	2.535	2.622	1.133				
1TMP	H6	15	2.584	2.464	1.084				
1TMP	H7	16	2.292	2.278	0.964				
1TMP	H8	17	2.466	2.306	0.964				
1TMP	H9	18	2.380	2.352	1.101				
1TMP	H10	19	2.100	2.454	0.762				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
3_chlorophenol									
13									
1TMP	C1	1	2.254	2.439	0.497				
1TMP	C2	2	2.158	2.334	0.475				
1TMP	C3	3	2.355	2.421	0.592				
1TMP	C4	4	2.253	2.204	0.653				
1TMP	C5	5	2.156	2.221	0.555				
1TMP	C6	6	2.359	2.303	0.668				
1TMP	O1	7	2.063	2.122	0.537				
1TMP	C11	8	2.472	2.279	0.791				
1TMP	H1	9	2.239	2.529	0.438				
1TMP	H2	10	2.087	2.349	0.394				
1TMP	H3	11	2.420	2.508	0.599				
1TMP	H4	12	2.245	2.120	0.721				
1TMP	H5	13	2.004	2.150	0.465				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
3_methoxyphenol									
17									
1TMP	C1	1	3.657	3.786	1.615				
1TMP	C2	2	3.764	3.725	1.550				
1TMP	C3	3	3.658	3.798	1.755				
1TMP	C4	4	3.871	3.685	1.763				
1TMP	C5	5	3.871	3.674	1.624				
1TMP	C6	6	3.764	3.747	1.828				
1TMP	C7	7	3.652	3.822	2.024				
1TMP	O1	8	3.975	3.613	1.561				
1TMP	O2	9	3.765	3.758	1.964				
1TMP	H1	10	3.574	3.826	1.558				
1TMP	H2	11	3.763	3.716	1.442				
1TMP	H3	12	3.574	3.846	1.805				
1TMP	H4	13	3.954	3.646	1.821				
1TMP	H5	14	3.574	3.749	2.043				
1TMP	H6	15	3.615	3.901	1.958				
1TMP	H7	16	3.684	3.867	2.119				
1TMP	H8	17	4.040	3.585	1.627				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
3_methylbutan_1_ol									
18									
1TMP	C1	1	3.846	3.737	1.918				
1TMP	C2	2	3.610	3.681	1.855				
1TMP	C3	3	3.788	3.713	1.675				
1TMP	C4	4	3.767	3.862	1.656				
1TMP	C5	5	3.757	3.663	1.817				
1TMP	O1	6	3.796	3.896	1.521				
1TMP	H1	7	3.829	3.701	2.020				

1TMP	H2	8	3.826	3.845	1.917				
1TMP	H3	9	3.952	3.722	1.895				
1TMP	H4	10	3.579	3.786	1.845				
1TMP	H5	11	3.593	3.651	1.959				
1TMP	H6	12	3.546	3.620	1.792				
1TMP	H7	13	3.724	3.659	1.603				
1TMP	H8	14	3.891	3.687	1.647				
1TMP	H9	15	3.663	3.890	1.677				
1TMP	H10	16	3.833	3.921	1.721				
1TMP	H11	17	3.783	3.557	1.824				
1TMP	H12	18	3.711	3.909	1.476				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
3_phenylpropanol									
22									
1TMP	C1	1	3.725	3.688	1.436				
1TMP	C2	2	3.618	3.748	1.503				
1TMP	C3	3	3.830	3.632	1.508				
1TMP	C4	4	3.616	3.751	1.643				
1TMP	C5	5	3.829	3.635	1.648				
1TMP	C6	6	3.721	3.694	1.715				
1TMP	C7	7	3.720	3.698	1.864				
1TMP	C8	8	3.787	3.823	1.920				
1TMP	C9	9	3.789	3.824	2.072				
1TMP	O1	10	3.852	3.944	2.117				
1TMP	H1	11	3.727	3.686	1.327				
1TMP	H2	12	3.536	3.792	1.447				
1TMP	H3	13	3.914	3.585	1.456				
1TMP	H4	14	3.533	3.798	1.694				
1TMP	H5	15	3.911	3.590	1.703				
1TMP	H6	16	3.770	3.608	1.905				
1TMP	H7	17	3.616	3.692	1.901				
1TMP	H8	18	3.737	3.913	1.884				
1TMP	H9	19	3.891	3.831	1.882				
1TMP	H10	20	3.688	3.821	2.113				
1TMP	H11	21	3.846	3.739	2.111				
1TMP	H12	22	3.842	4.009	2.046				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
benzyl_alcohol									
16									
1TMP	C1	1	3.748	3.732	1.548				
1TMP	C2	2	3.641	3.792	1.615				
1TMP	C3	3	3.853	3.676	1.620				
1TMP	C4	4	3.639	3.795	1.755				
1TMP	C5	5	3.851	3.679	1.760				
1TMP	C6	6	3.744	3.738	1.827				
1TMP	C7	7	3.742	3.742	1.976				
1TMP	O1	8	3.806	3.860	2.022				
1TMP	H1	9	3.749	3.730	1.439				
1TMP	H2	10	3.559	3.836	1.559				
1TMP	H3	11	3.936	3.629	1.568				
1TMP	H4	12	3.555	3.842	1.806				
1TMP	H5	13	3.933	3.634	1.815				
1TMP	H6	14	3.640	3.740	2.015				
1TMP	H7	15	3.795	3.655	2.018				
1TMP	H8	16	3.806	3.922	1.947				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
butan_1_ol									
15									
1TMP	C1	1	3.935	3.853	1.752				
1TMP	C2	2	3.837	3.756	1.815				
1TMP	C3	3	3.702	3.759	1.744				
1TMP	C4	4	3.605	3.658	1.804				
1TMP	O1	5	3.482	3.665	1.733				
1TMP	H1	6	3.953	3.828	1.647				
1TMP	H2	7	3.898	3.955	1.757				
1TMP	H3	8	4.032	3.849	1.804				
1TMP	H4	9	3.879	3.654	1.811				
1TMP	H5	10	3.824	3.781	1.921				
1TMP	H6	11	3.658	3.859	1.750				
1TMP	H7	12	3.715	3.737	1.637				
1TMP	H8	13	3.644	3.557	1.797				
1TMP	H9	14	3.585	3.681	1.910				

1TMP	H10	15	3.504	3.664	1.639					
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000	
butan_2_ol										
15										
1TMP	C1	1	3.762	3.700	1.963					
1TMP	C2	2	3.770	3.797	1.588					
1TMP	C3	3	3.805	3.771	1.836					
1TMP	C4	4	3.728	3.722	1.713					
1TMP	O1	5	3.588	3.742	1.734					
1TMP	H1	6	3.777	3.592	1.955					
1TMP	H2	7	3.656	3.718	1.986					
1TMP	H3	8	3.821	3.736	2.048					
1TMP	H4	9	3.749	3.904	1.597					
1TMP	H5	10	3.877	3.784	1.567					
1TMP	H6	11	3.714	3.762	1.501					
1TMP	H7	12	3.912	3.755	1.821					
1TMP	H8	13	3.789	3.878	1.850					
1TMP	H9	14	3.745	3.614	1.699					
1TMP	H10	15	3.554	3.782	1.653					
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000	
cycloheptanol										
22										
1TMP	C1	1	3.907	3.684	1.796					
1TMP	C2	2	3.905	3.832	1.833					
1TMP	C3	3	3.833	3.649	1.667					
1TMP	C4	4	3.777	3.909	1.806					
1TMP	C5	5	3.684	3.624	1.689					
1TMP	C6	6	3.648	3.834	1.836					
1TMP	C7	7	3.600	3.749	1.718					
1TMP	O1	8	3.467	3.706	1.747					
1TMP	H1	9	4.012	3.654	1.786					
1TMP	H2	10	3.867	3.625	1.879					
1TMP	H3	11	3.930	3.840	1.940					
1TMP	H4	12	3.987	3.883	1.781					
1TMP	H5	13	3.849	3.726	1.590					
1TMP	H6	14	3.877	3.556	1.628					
1TMP	H7	15	3.779	4.000	1.868					
1TMP	H8	16	3.776	3.945	1.702					
1TMP	H9	17	3.643	3.576	1.600					
1TMP	H10	18	3.671	3.551	1.770					
1TMP	H11	19	3.657	3.773	1.926					
1TMP	H12	20	3.569	3.907	1.858					
1TMP	H13	21	3.595	3.810	1.627					
1TMP	H14	22	3.470	3.665	1.835					
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000	
cyclohexanol										
19										
1TMP	C1	1	3.633	3.632	1.786					
1TMP	C2	2	3.747	3.642	1.887					
1TMP	C3	3	3.675	3.685	1.648					
1TMP	C4	4	3.803	3.784	1.896					
1TMP	C5	5	3.730	3.827	1.657					
1TMP	C6	6	3.845	3.836	1.759					
1TMP	O1	7	3.887	3.971	1.770					
1TMP	H1	8	3.600	3.528	1.777					
1TMP	H2	9	3.547	3.690	1.822					
1TMP	H3	10	3.711	3.610	1.985					
1TMP	H4	11	3.827	3.573	1.858					
1TMP	H5	12	3.751	3.619	1.605					
1TMP	H6	13	3.589	3.683	1.580					
1TMP	H7	14	3.727	3.851	1.940					
1TMP	H8	15	3.888	3.786	1.964					
1TMP	H9	16	3.765	3.860	1.559					
1TMP	H10	17	3.650	3.897	1.685					
1TMP	H11	18	3.930	3.778	1.722					
1TMP	H12	19	3.941	3.991	1.692					
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000	
cyclopentanol										
16										
1TMP	C1	1	3.794	3.618	1.749					
1TMP	C2	2	3.877	3.720	1.825					
1TMP	C3	3	3.710	3.704	1.655					

1TMP	C4	4	3.783	3.840	1.845				
1TMP	C5	5	3.672	3.824	1.741				
1TMP	O1	6	3.548	3.799	1.807				
1TMP	H1	7	3.857	3.546	1.694				
1TMP	H2	8	3.730	3.562	1.817				
1TMP	H3	9	3.914	3.681	1.920				
1TMP	H4	10	3.963	3.751	1.765				
1TMP	H5	11	3.772	3.737	1.571				
1TMP	H6	12	3.624	3.649	1.617				
1TMP	H7	13	3.744	3.841	1.947				
1TMP	H8	14	3.839	3.933	1.829				
1TMP	H9	15	3.658	3.914	1.681				
1TMP	H10	16	3.508	3.885	1.826				
5.00000	5.00000	3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000	

decan\_1\_ol  
33

1TMP	C1	1	3.883	4.107	2.223				
1TMP	C2	2	3.840	4.090	2.078				
1TMP	C3	3	3.840	3.943	2.036				
1TMP	C4	4	3.794	3.926	1.891				
1TMP	C5	5	3.791	3.778	1.851				
1TMP	C6	6	3.739	3.755	1.709				
1TMP	C7	7	3.729	3.607	1.672				
1TMP	C8	8	3.679	3.589	1.528				
1TMP	C9	9	3.666	3.441	1.491				
1TMP	C10	10	3.613	3.421	1.350				
1TMP	O1	11	3.605	3.282	1.320				
1TMP	H1	12	3.984	4.069	2.238				
1TMP	H2	13	3.815	4.053	2.290				
1TMP	H3	14	3.882	4.213	2.250				
1TMP	H4	15	3.740	4.132	2.065				
1TMP	H5	16	3.908	4.147	2.013				
1TMP	H6	17	3.942	3.902	2.047				
1TMP	H7	18	3.775	3.886	2.103				
1TMP	H8	19	3.862	3.981	1.825				
1TMP	H9	20	3.694	3.969	1.879				
1TMP	H10	21	3.892	3.735	1.861				
1TMP	H11	22	3.726	3.723	1.921				
1TMP	H12	23	3.803	3.807	1.637				
1TMP	H13	24	3.639	3.800	1.702				
1TMP	H14	25	3.660	3.556	1.741				
1TMP	H15	26	3.827	3.559	1.682				
1TMP	H16	27	3.748	3.638	1.459				
1TMP	H17	28	3.582	3.639	1.517				
1TMP	H18	29	3.763	3.392	1.500				
1TMP	H19	30	3.598	3.393	1.563				
1TMP	H20	31	3.681	3.467	1.278				
1TMP	H21	32	3.513	3.466	1.338				
1TMP	H22	33	3.527	3.270	1.263				

5.00000 5.00000 3.53553 0.00000 0.00000 0.00000 0.00000 2.50000 2.50000  
ethanol  
9

1TMP	C1	1	3.701	3.683	1.816				
1TMP	C2	2	3.786	3.801	1.774				
1TMP	O1	3	3.747	3.842	1.644				
1TMP	H1	4	3.729	3.649	1.916				
1TMP	H2	5	3.595	3.710	1.816				
1TMP	H3	6	3.713	3.600	1.746				
1TMP	H4	7	3.892	3.774	1.771				
1TMP	H5	8	3.772	3.885	1.843				
1TMP	H6	9	3.811	3.804	1.581				

5.00000 5.00000 3.53553 0.00000 0.00000 0.00000 0.00000 2.50000 2.50000  
heptan\_1\_ol  
24

1TMP	C1	1	4.033	3.847	2.036				
1TMP	C2	2	3.992	3.801	1.897				
1TMP	C3	3	3.840	3.800	1.882				
1TMP	C4	4	3.792	3.748	1.746				
1TMP	C5	5	3.640	3.740	1.733				
1TMP	C6	6	3.599	3.685	1.597				
1TMP	C7	7	3.447	3.681	1.582				
1TMP	O1	8	3.415	3.631	1.453				

1TMP	H1	9	3.997	3.948	2.057				
1TMP	H2	10	4.142	3.847	2.045				
1TMP	H3	11	3.993	3.780	2.113				
1TMP	H4	12	4.032	3.701	1.879				
1TMP	H5	13	4.037	3.868	1.823				
1TMP	H6	14	3.800	3.901	1.898				
1TMP	H7	15	3.796	3.737	1.960				
1TMP	H8	16	3.833	3.811	1.666				
1TMP	H9	17	3.835	3.648	1.731				
1TMP	H10	18	3.596	3.840	1.747				
1TMP	H11	19	3.600	3.676	1.812				
1TMP	H12	20	3.639	3.585	1.582				
1TMP	H13	21	3.641	3.747	1.517				
1TMP	H14	22	3.404	3.781	1.591				
1TMP	H15	23	3.402	3.615	1.657				
1TMP	H16	24	3.496	3.588	1.418				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
hexan_1_ol									
21									
1TMP	C1	1	3.990	3.738	1.530				
1TMP	C2	2	3.926	3.685	1.657				
1TMP	C3	3	3.800	3.763	1.693				
1TMP	C4	4	3.735	3.719	1.824				
1TMP	C5	5	3.607	3.795	1.858				
1TMP	C6	6	3.549	3.750	1.991				
1TMP	O1	7	3.430	3.823	2.017				
1TMP	H1	8	4.081	3.681	1.506				
1TMP	H2	9	3.922	3.730	1.445				
1TMP	H3	10	4.019	3.843	1.541				
1TMP	H4	11	3.999	3.693	1.739				
1TMP	H5	12	3.903	3.579	1.643				
1TMP	H6	13	3.727	3.754	1.611				
1TMP	H7	14	3.825	3.870	1.701				
1TMP	H8	15	3.808	3.734	1.905				
1TMP	H9	16	3.714	3.611	1.820				
1TMP	H10	17	3.532	3.781	1.780				
1TMP	H11	18	3.627	3.903	1.862				
1TMP	H12	19	3.524	3.643	1.989				
1TMP	H13	20	3.619	3.768	2.073				
1TMP	H14	21	3.416	3.881	1.940				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
hexan_3_ol									
21									
1TMP	C1	1	3.732	3.585	1.513				
1TMP	C2	2	3.718	3.834	2.053				
1TMP	C3	3	3.765	3.627	1.655				
1TMP	C4	4	3.693	3.784	1.912				
1TMP	C5	5	3.771	3.780	1.668				
1TMP	C6	6	3.802	3.825	1.811				
1TMP	O1	7	3.812	3.967	1.813				
1TMP	H1	8	3.635	3.624	1.482				
1TMP	H2	9	3.808	3.621	1.443				
1TMP	H3	10	3.728	3.476	1.506				
1TMP	H4	11	3.733	3.942	2.055				
1TMP	H5	12	3.632	3.810	2.117				
1TMP	H6	13	3.806	3.786	2.098				
1TMP	H7	14	3.689	3.587	1.723				
1TMP	H8	15	3.861	3.583	1.684				
1TMP	H9	16	3.597	3.823	1.877				
1TMP	H10	17	3.682	3.675	1.912				
1TMP	H11	18	3.849	3.818	1.600				
1TMP	H12	19	3.676	3.822	1.635				
1TMP	H13	20	3.899	3.784	1.843				
1TMP	H14	21	3.860	3.992	1.732				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
m_cresol									
16									
1TMP	C1	1	2.464	1.789	0.949				
1TMP	C2	2	2.509	1.892	1.031				
1TMP	C3	3	2.518	1.772	0.819				
1TMP	C4	4	2.691	1.928	0.876				
1TMP	C5	5	2.627	1.953	0.996				

1TMP	C6	6	2.631	1.840	0.783				
1TMP	C7	7	2.677	2.054	1.094				
1TMP	O1	8	2.689	1.814	0.658				
1TMP	H1	9	2.377	1.731	0.980				
1TMP	H2	10	2.459	1.920	1.123				
1TMP	H3	11	2.470	1.706	0.748				
1TMP	H4	12	2.782	1.981	0.851				
1TMP	H5	13	2.773	2.019	1.132				
1TMP	H6	14	2.685	2.157	1.058				
1TMP	H7	15	2.614	2.065	1.182				
1TMP	H8	16	2.771	1.867	0.655				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
methanol									
6									
1TMP	C1	1	3.757	3.721	1.790				
1TMP	O1	2	3.698	3.844	1.754				
1TMP	H1	3	3.722	3.691	1.890				
1TMP	H2	4	3.866	3.731	1.790				
1TMP	H3	5	3.728	3.645	1.718				
1TMP	H4	6	3.731	3.867	1.666				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
nonan_1_ol									
30									
1TMP	C1	1	3.805	3.477	2.220				
1TMP	C2	2	3.749	3.488	2.079				
1TMP	C3	3	3.780	3.625	2.018				
1TMP	C4	4	3.734	3.638	1.872				
1TMP	C5	5	3.767	3.770	1.803				
1TMP	C6	6	3.721	3.776	1.657				
1TMP	C7	7	3.759	3.910	1.592				
1TMP	C8	8	3.715	3.915	1.446				
1TMP	C9	9	3.750	4.048	1.380				
1TMP	O1	10	3.706	4.048	1.245				
1TMP	H1	11	3.781	3.379	2.263				
1TMP	H2	12	3.913	3.490	2.221				
1TMP	H3	13	3.761	3.554	2.286				
1TMP	H4	14	3.641	3.471	2.083				
1TMP	H5	15	3.793	3.409	2.017				
1TMP	H6	16	3.735	3.704	2.078				
1TMP	H7	17	3.888	3.642	2.020				
1TMP	H8	18	3.625	3.622	1.868				
1TMP	H9	19	3.779	3.556	1.814				
1TMP	H10	20	3.718	3.851	1.859				
1TMP	H11	21	3.874	3.790	1.809				
1TMP	H12	22	3.612	3.763	1.652				
1TMP	H13	23	3.766	3.695	1.600				
1TMP	H14	24	3.712	3.992	1.647				
1TMP	H15	25	3.867	3.924	1.600				
1TMP	H16	26	3.765	3.833	1.391				
1TMP	H17	27	3.607	3.899	1.439				
1TMP	H18	28	3.700	4.130	1.432				
1TMP	H19	29	3.858	4.065	1.382				
1TMP	H20	30	3.609	4.048	1.247				
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
o_cresol									
16									
1TMP	C1	1	1.961	2.223	1.469				
1TMP	C2	2	2.093	2.272	1.480				
1TMP	C3	3	1.903	2.182	1.343				
1TMP	C4	4	2.168	2.273	1.360				
1TMP	C5	5	1.975	2.184	1.224				
1TMP	C6	6	2.105	2.235	1.236				
1TMP	C7	7	1.909	2.142	1.093				
1TMP	O1	8	2.174	2.258	1.123				
1TMP	H1	9	1.897	2.225	1.557				
1TMP	H2	10	2.144	2.278	1.576				
1TMP	H3	11	1.804	2.138	1.339				
1TMP	H4	12	2.268	2.317	1.360				
1TMP	H5	13	1.936	2.212	1.014				
1TMP	H6	14	1.949	2.047	1.057				
1TMP	H7	15	1.801	2.130	1.105				
1TMP	H8	16	2.224	2.341	1.133				

5.00000	5.00000	3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
octan_1_ol								
27								
1TMP	C1	1	4.039	4.038	1.996			
1TMP	C2	2	3.985	3.898	1.968			
1TMP	C3	3	3.867	3.902	1.871			
1TMP	C4	4	3.816	3.761	1.840			
1TMP	C5	5	3.702	3.759	1.738			
1TMP	C6	6	3.656	3.618	1.701			
1TMP	C7	7	3.544	3.622	1.597			
1TMP	C8	8	3.495	3.482	1.563			
1TMP	O1	9	3.392	3.492	1.465			
1TMP	H1	10	3.962	4.101	2.041			
1TMP	H2	11	4.074	4.086	1.904			
1TMP	H3	12	4.123	4.032	2.066			
1TMP	H4	13	3.955	3.851	2.062			
1TMP	H5	14	4.066	3.837	1.926			
1TMP	H6	15	3.787	3.962	1.915			
1TMP	H7	16	3.897	3.952	1.778			
1TMP	H8	17	3.784	3.712	1.932			
1TMP	H9	18	3.899	3.702	1.800			
1TMP	H10	19	3.617	3.817	1.776			
1TMP	H11	20	3.737	3.810	1.647			
1TMP	H12	21	3.620	3.565	1.790			
1TMP	H13	22	3.741	3.561	1.661			
1TMP	H14	23	3.579	3.671	1.505			
1TMP	H15	24	3.460	3.682	1.634			
1TMP	H16	25	3.576	3.421	1.522			
1TMP	H17	26	3.454	3.432	1.651			
1TMP	H18	27	3.433	3.474	1.379			
5.00000	5.00000	3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
p_cresol								
16								
1TMP	C1	1	3.649	3.803	1.738			
1TMP	C2	2	3.861	3.687	1.744			
1TMP	C3	3	3.647	3.806	1.878			
1TMP	C4	4	3.859	3.690	1.883			
1TMP	C5	5	3.756	3.744	1.671			
1TMP	C6	6	3.752	3.750	1.950			
1TMP	C7	7	3.758	3.740	1.522			
1TMP	O1	8	3.750	3.753	2.086			
1TMP	H1	9	3.567	3.847	1.683			
1TMP	H2	10	3.944	3.641	1.693			
1TMP	H3	11	3.563	3.853	1.930			
1TMP	H4	12	3.941	3.647	1.939			
1TMP	H5	13	3.777	3.638	1.487			
1TMP	H6	14	3.662	3.774	1.480			
1TMP	H7	15	3.835	3.807	1.482			
1TMP	H8	16	3.685	3.819	2.115			
5.00000	5.00000	3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
pentan_1_ol								
18								
1TMP	C1	1	3.583	3.839	1.967			
1TMP	C2	2	3.663	3.733	1.893			
1TMP	C3	3	3.730	3.790	1.768			
1TMP	C4	4	3.813	3.684	1.696			
1TMP	C5	5	3.884	3.741	1.575			
1TMP	O1	6	3.961	3.638	1.513			
1TMP	H1	7	3.647	3.921	1.999			
1TMP	H2	8	3.504	3.880	1.903			
1TMP	H3	9	3.536	3.796	2.056			
1TMP	H4	10	3.596	3.651	1.865			
1TMP	H5	11	3.739	3.691	1.961			
1TMP	H6	12	3.654	3.830	1.700			
1TMP	H7	13	3.795	3.874	1.797			
1TMP	H8	14	3.749	3.601	1.665			
1TMP	H9	15	3.888	3.641	1.765			
1TMP	H10	16	3.952	3.822	1.603			
1TMP	H11	17	3.812	3.779	1.502			
1TMP	H12	18	3.992	3.581	1.585			
5.00000	5.00000	3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000
pentan_2_ol								

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18
1TMP    C1     1   3.747  3.911  1.980
1TMP    C2     2   3.708  3.554  1.625
1TMP    C3     3   3.795  3.865  1.844
1TMP    C4     4   3.731  3.731  1.804
1TMP    C5     5   3.775  3.685  1.665
1TMP    O1     6   3.743  3.784  1.568
1TMP    H1     7   3.794  4.007  2.006
1TMP    H2     8   3.772  3.838  2.058
1TMP    H3     9   3.638  3.926  1.981
1TMP    H4    10   3.599  3.566  1.622
1TMP    H5    11   3.739  3.524  1.525
1TMP    H6    12   3.732  3.474  1.696
1TMP    H7    13   3.771  3.941  1.769
1TMP    H8    14   3.904  3.854  1.846
1TMP    H9    15   3.757  3.655  1.879
1TMP    H10   16   3.622  3.743  1.806
1TMP    H11   17   3.884  3.671  1.663
1TMP    H12   18   3.797  3.764  1.490
5.00000  5.00000  3.53553  0.00000  0.00000  0.00000  0.00000  2.50000  2.50000
pentan_3_ol
18
1TMP    C1     1   3.855  3.800  1.542
1TMP    C2     2   3.604  3.680  1.968
1TMP    C3     3   3.833  3.829  1.690
1TMP    C4     4   3.708  3.769  1.901
1TMP    C5     5   3.725  3.739  1.752
1TMP    O1     6   3.763  3.603  1.734
1TMP    H1     7   3.931  3.868  1.501
1TMP    H2     8   3.890  3.697  1.527
1TMP    H3     9   3.763  3.813  1.485
1TMP    H4    10   3.591  3.710  2.072
1TMP    H5    11   3.507  3.689  1.918
1TMP    H6    12   3.634  3.575  1.967
1TMP    H7    13   3.928  3.814  1.743
1TMP    H8    14   3.805  3.934  1.701
1TMP    H9    15   3.804  3.755  1.953
1TMP    H10   16   3.679  3.874  1.915
1TMP    H11   17   3.630  3.755  1.699
1TMP    H12   18   3.858  3.598  1.755
5.00000  5.00000  3.53553  0.00000  0.00000  0.00000  0.00000  2.50000  2.50000
phenol
13
1TMP    C1     1   3.757  3.741  1.603
1TMP    C2     2   3.650  3.801  1.670
1TMP    C3     3   3.862  3.685  1.675
1TMP    C4     4   3.648  3.804  1.810
1TMP    C5     5   3.860  3.688  1.815
1TMP    C6     6   3.753  3.747  1.882
1TMP    O1     7   3.751  3.750  2.018
1TMP    H1     8   3.758  3.739  1.494
1TMP    H2     9   3.568  3.845  1.614
1TMP    H3    10   3.945  3.638  1.623
1TMP    H4    11   3.565  3.851  1.862
1TMP    H5    12   3.942  3.643  1.871
1TMP    H6    13   3.686  3.816  2.047
5.00000  5.00000  3.53553  0.00000  0.00000  0.00000  0.00000  2.50000  2.50000
prop_2_en_1_ol
10
1TMP    C1     1   3.855  3.852  1.721
1TMP    C2     2   3.743  3.811  1.781
1TMP    C3     3   3.675  3.682  1.750
1TMP    O1     4   3.671  3.602  1.868
1TMP    H1     5   3.902  3.947  1.747
1TMP    H2     6   3.902  3.792  1.644
1TMP    H3     7   3.698  3.874  1.857
1TMP    H4     8   3.727  3.625  1.672
1TMP    H5     9   3.572  3.701  1.718
1TMP    H6    10   3.754  3.618  1.916
5.00000  5.00000  3.53553  0.00000  0.00000  0.00000  0.00000  2.50000  2.50000
propan_1_ol
12

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1TMP	C1	1	3.647	3.770	1.659					
1TMP	C2	2	3.771	3.792	1.743					
1TMP	C3	3	3.775	3.701	1.865					
1TMP	O1	4	3.893	3.727	1.939					
1TMP	H1	5	3.556	3.789	1.717					
1TMP	H2	6	3.647	3.836	1.572					
1TMP	H3	7	3.641	3.665	1.623					
1TMP	H4	8	3.777	3.895	1.774					
1TMP	H5	9	3.861	3.773	1.682					
1TMP	H6	10	3.688	3.718	1.929					
1TMP	H7	11	3.775	3.595	1.835					
1TMP	H8	12	3.965	3.737	1.874					
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000	
propan_2_ol										
12										
1TMP	C1	1	3.685	3.672	1.687					
1TMP	C2	2	3.861	3.771	1.837					
1TMP	C3	3	3.712	3.759	1.808					
1TMP	O1	4	3.658	3.889	1.786					
1TMP	H1	5	3.722	3.570	1.701					
1TMP	H2	6	3.577	3.667	1.667					
1TMP	H3	7	3.731	3.714	1.597					
1TMP	H4	8	3.906	3.673	1.857					
1TMP	H5	9	3.878	3.836	1.923					
1TMP	H6	10	3.914	3.817	1.752					
1TMP	H7	11	3.662	3.717	1.896					
1TMP	H8	12	3.690	3.918	1.700					
5.00000	5.00000		3.53553	0.00000	0.00000	0.00000	0.00000	2.50000	2.50000	

**Partial charges used for GAFF/AM1-BCC (column 3) and GAFF/AM1-BCC DC (column 4).**

12_ethanediol			
1	C1	0.0977000	0.1181200
2	C2	0.0977000	0.1181200
3	O1	-0.5999000	-0.7253000
4	O2	-0.5997000	-0.7250600
5	H1	0.0486000	0.0587600
6	H2	0.0486000	0.0587600
7	H3	0.0486000	0.0587600
8	H4	0.0486000	0.0587600
9	H5	0.4049000	0.4895400
10	H6	0.4049000	0.4895400
13_propanediol			
1	O1	-0.5983010	-0.7233800
2	C1	0.1324000	0.1600800
3	C2	-0.0884000	-0.0773200
4	C3	0.1324000	0.1600800
5	O2	-0.5983010	-0.7233800
6	H12	0.0197000	0.0238200
7	H13	0.0197000	0.0238200
8	H22	0.0707000	0.0707000
9	H23	0.0707000	0.0707000
10	H32	0.0197000	0.0238200
11	H33	0.0197000	0.0238200
12	HO2	0.4000000	0.4836200
13	HO1	0.4000000	0.4836200
2_butoxyethanol			
1	C1	-0.0907000	-0.0907000
2	C2	-0.0769000	-0.0769000
3	C3	-0.0800000	-0.0800000
4	C4	0.1348000	0.1347994
5	C5	0.1310000	0.1583894
6	C6	0.0959000	0.0869094
7	O1	-0.5982000	-0.7232500
8	O2	-0.4295000	-0.4295000
9	H1	0.0326000	0.0325994
10	H2	0.0326000	0.0325994
11	H3	0.0326000	0.0325994
12	H4	0.0413000	0.0412994
13	H5	0.0413000	0.0412994
14	H6	0.0520000	0.0519994
15	H7	0.0520000	0.0519994
16	H8	0.0262000	0.0261994
17	H9	0.0262000	0.0261994
18	H10	0.0530000	0.0640794
19	H11	0.0530000	0.0640794
20	H12	0.0333000	0.0332994
21	H13	0.0333000	0.0332994
22	H14	0.4042000	0.4886994
2_chlorophenol			
1	C1	-0.0940000	-0.0940000
2	C2	-0.1589000	-0.1589000
3	C3	-0.1515000	-0.1594200
4	C4	-0.0850000	-0.0850000
5	C5	0.1372000	0.1658783
6	C6	-0.0711000	-0.0790200
7	O1	-0.4921000	-0.5949700
8	C11	-0.0965000	-0.0965000
9	H1	0.1387000	0.1386983
10	H2	0.1395000	0.1394983
11	H3	0.1553000	0.1552983
12	H4	0.1477000	0.1476983
13	H5	0.4307000	0.5207383
2_ethoxyethanol			
1	C1	-0.1100000	-0.1100000
2	C2	0.1322000	0.1322000
3	C3	0.1265000	0.1529400
4	C4	0.1035000	0.0991500
5	O1	-0.6026000	-0.7285700
6	O2	-0.4314000	-0.4314000

7	H1	0.0435000	0.0435000
8	H2	0.0435000	0.0435000
9	H3	0.0435000	0.0435000
10	H4	0.0352000	0.0352000
11	H5	0.0352000	0.0352000
12	H6	0.0438000	0.0529600
13	H7	0.0438000	0.0529600
14	H8	0.0420000	0.0420000
15	H9	0.0420000	0.0420000
16	H10	0.4093000	0.4948600
2_methoxyethanol			
1	C1	0.1178000	0.1177989
2	C2	0.1112000	0.1344489
3	C3	0.1908000	0.2095489
4	O1	-0.6000000	-0.7254300
5	O2	-0.4212000	-0.4212000
6	H1	0.0333000	0.0332989
7	H2	0.0333000	0.0332989
8	H3	0.0333000	0.0332989
9	H4	-0.0026000	-0.0031400
10	H5	-0.0026000	-0.0031400
11	H6	0.0512000	0.0511989
12	H7	0.0512000	0.0511989
13	H8	0.4043000	0.4888189
2_methylbutan_1_ol			
1	C1	-0.0910000	-0.0909980
2	C2	-0.0876000	-0.0875980
3	C3	-0.0732000	-0.0731980
4	C4	0.1342000	0.1622500
5	C5	-0.0952000	-0.0967880
6	O1	-0.6004000	-0.7259080
7	H1	0.0341000	0.0341000
8	H2	0.0341000	0.0341000
9	H3	0.0341000	0.0341000
10	H4	0.0362000	0.0362000
11	H5	0.0362000	0.0362000
12	H6	0.0362000	0.0362000
13	H7	0.0392000	0.0392000
14	H8	0.0392000	0.0392000
15	H9	0.0381000	0.0460600
16	H10	0.0381000	0.0460600
17	H11	0.0501000	0.0501000
18	H12	0.3976000	0.4807200
2_methylbutan_2_ol			
1	C1	-0.0889000	-0.0888999
2	C2	-0.1201000	-0.1162999
3	C3	-0.1201000	-0.1162999
4	C4	-0.0638000	-0.0599999
5	C5	0.1499000	0.1812392
6	O1	-0.6029000	-0.7289399
7	H1	0.0356000	0.0355992
8	H2	0.0356000	0.0355992
9	H3	0.0356000	0.0355992
10	H4	0.0408000	0.0407992
11	H5	0.0408000	0.0407992
12	H6	0.0408000	0.0407992
13	H7	0.0408000	0.0407992
14	H8	0.0408000	0.0407992
15	H9	0.0408000	0.0407992
16	H10	0.0479000	0.0478992
17	H11	0.0479000	0.0478992
18	H12	0.3985000	0.4818092
2_methylpropan_1_ol			
1	C1	-0.0862000	-0.0861975
2	C2	-0.0862000	-0.0861975
3	C3	0.1366000	0.1651600
4	C4	-0.0656000	-0.0595375
5	O1	-0.6021000	-0.7279675
6	H1	0.0361000	0.0361000
7	H2	0.0361000	0.0361000
8	H3	0.0361000	0.0361000
9	H4	0.0361000	0.0361000

10	H5	0.0361000	0.0361000
11	H6	0.0361000	0.0361000
12	H7	0.0191000	0.0230900
13	H8	0.0191000	0.0230900
14	H9	0.0504000	0.0504000
15	H10	0.3983000	0.4815600
2_methylpropan_2_ol			
1	C1	-0.1062000	-0.1021875
2	C2	-0.1062000	-0.1021875
3	C3	-0.1062000	-0.1021875
4	C4	0.1467000	0.1773700
5	O1	-0.6013000	-0.7269975
6	H1	0.0418000	0.0418000
7	H2	0.0418000	0.0418000
8	H3	0.0418000	0.0418000
9	H4	0.0418000	0.0418000
10	H5	0.0418000	0.0418000
11	H6	0.0418000	0.0418000
12	H7	0.0418000	0.0418000
13	H8	0.0418000	0.0418000
14	H9	0.0418000	0.0418000
15	H10	0.3970000	0.4799900
2_phenylethanol			
1	C1	-0.1309000	-0.1309000
2	C2	-0.1296000	-0.1296000
3	C3	-0.1296000	-0.1296000
4	C4	-0.1236000	-0.1236000
5	C5	-0.1236000	-0.1236000
6	C6	-0.0693000	-0.0693000
7	C7	-0.0565000	-0.0551200
8	C8	0.1367000	0.1652782
9	O1	-0.6014000	-0.7271200
10	H1	0.1303000	0.1302982
11	H2	0.1304000	0.1303982
12	H3	0.1304000	0.1303982
13	H4	0.1322000	0.1321982
14	H5	0.1322000	0.1321982
15	H6	0.0571000	0.0570982
16	H7	0.0571000	0.0570982
17	H8	0.0293000	0.0354282
18	H9	0.0293000	0.0354282
19	H10	0.3995000	0.4830182
222_trifluoroethanol			
1	C1	0.0976000	0.1180000
2	C2	0.6491000	0.6356000
3	O1	-0.5785000	-0.6994375
4	F1	-0.2379000	-0.2378975
5	F2	-0.2379000	-0.2378975
6	F3	-0.2379000	-0.2378975
7	H1	0.0620000	0.0749600
8	H2	0.0620000	0.0749600
9	H3	0.4215000	0.5096100
23_dimethylphenol			
1	C1	-0.0938000	-0.0938000
2	C2	-0.1613000	-0.1613000
3	C3	-0.2148000	-0.2192200
4	C4	-0.0383000	-0.0383000
5	C5	-0.0907000	-0.0951200
6	C6	0.1259000	0.1522191
7	C7	-0.0616000	-0.0616000
8	C8	-0.0522000	-0.0522000
9	O1	-0.5020000	-0.6069400
10	H1	0.1316000	0.1315991
11	H2	0.1324000	0.1323991
12	H3	0.1316000	0.1315991
13	H4	0.0449000	0.0448991
14	H5	0.0449000	0.0448991
15	H6	0.0449000	0.0448991
16	H7	0.0467000	0.0466991
17	H8	0.0467000	0.0466991
18	H9	0.0467000	0.0466991
19	H10	0.4184000	0.5058691

3_chlorophenol			
1	C1	-0.0889000	-0.0889000
2	C2	-0.1565000	-0.1629600
3	C3	-0.1601000	-0.1601000
4	C4	-0.2123000	-0.2187600
5	C5	0.1344000	0.1625000
6	C6	0.0558000	0.0558000
7	O1	-0.4953000	-0.5988400
8	Cl1	-0.0922000	-0.0922000
9	H1	0.1404000	0.1404000
10	H2	0.1544000	0.1544000
11	H3	0.1492000	0.1492000
12	H4	0.1484000	0.1484000
13	H5	0.4227000	0.5110600
3_methoxyphenol			
1	C1	-0.0602000	-0.0601983
2	C2	-0.2481000	-0.2563483
3	C3	-0.2146000	-0.2145983
4	C4	-0.2111000	-0.2193483
5	C5	0.1559000	0.1884900
6	C6	0.1570000	0.1570000
7	C7	0.1167000	0.1167000
8	O1	-0.4981000	-0.6022283
9	O2	-0.3266000	-0.3265983
10	H1	0.1340000	0.1340000
11	H2	0.1345000	0.1345000
12	H3	0.1446000	0.1446000
13	H4	0.1608000	0.1608000
14	H5	0.0447000	0.0447000
15	H6	0.0447000	0.0447000
16	H7	0.0447000	0.0447000
17	H8	0.4211000	0.5091300
3_methylbutan_1_ol			
1	C1	-0.0882000	-0.0882000
2	C2	-0.0882000	-0.0882000
3	C3	-0.0977000	-0.0965100
4	C4	0.1317000	0.1592300
5	C5	-0.0641000	-0.0641000
6	O1	-0.6024000	-0.7283300
7	H1	0.0336000	0.0336000
8	H2	0.0336000	0.0336000
9	H3	0.0336000	0.0336000
10	H4	0.0336000	0.0336000
11	H5	0.0336000	0.0336000
12	H6	0.0336000	0.0336000
13	H7	0.0469000	0.0469000
14	H8	0.0469000	0.0469000
15	H9	0.0339000	0.0409900
16	H10	0.0339000	0.0409900
17	H11	0.0485000	0.0485000
18	H12	0.3972000	0.4802300
3_phenylpropanol			
1	C1	-0.1314000	-0.1314000
2	C2	-0.1276000	-0.1276000
3	C3	-0.1276000	-0.1276000
4	C4	-0.1282000	-0.1282000
5	C5	-0.1282000	-0.1282000
6	C6	-0.0731000	-0.0731000
7	C7	-0.0446000	-0.0446000
8	C8	-0.1057000	-0.1074100
9	C9	0.1313000	0.1587500
10	O1	-0.6014000	-0.7271200
11	H1	0.1312000	0.1312000
12	H2	0.1313000	0.1313000
13	H3	0.1313000	0.1313000
14	H4	0.1321000	0.1321000
15	H5	0.1321000	0.1321000
16	H6	0.0503000	0.0503000
17	H7	0.0503000	0.0503000
18	H8	0.0498000	0.0498000
19	H9	0.0498000	0.0498000
20	H10	0.0391000	0.0472700

21	H11	0.0391000	0.0472700
22	H12	0.4001000	0.4837400
benzyl_alcohol			
1	C1	-0.1215000	-0.1214986
2	C2	-0.1327000	-0.1326986
3	C3	-0.1327000	-0.1326986
4	C4	-0.1125000	-0.1124986
5	C5	-0.1125000	-0.1124986
6	C6	-0.1266000	-0.1413986
7	C7	0.1670000	0.2019100
8	O1	-0.5964000	-0.7210786
9	H1	0.1325000	0.1325000
10	H2	0.1331000	0.1331000
11	H3	0.1331000	0.1331000
12	H4	0.1345000	0.1345000
13	H5	0.1345000	0.1345000
14	H6	0.0491000	0.0593600
15	H7	0.0491000	0.0593600
16	H8	0.4020000	0.4860400
butan_1_ol			
1	C1	-0.0924000	-0.0923975
2	C2	-0.0763000	-0.0762975
3	C3	-0.1125000	-0.1140275
4	C4	0.1307000	0.1580200
5	O1	-0.6011000	-0.7267575
6	H1	0.0341000	0.0341000
7	H2	0.0341000	0.0341000
8	H3	0.0341000	0.0341000
9	H4	0.0397000	0.0397000
10	H5	0.0397000	0.0397000
11	H6	0.0461000	0.0461000
12	H7	0.0461000	0.0461000
13	H8	0.0402000	0.0486000
14	H9	0.0402000	0.0486000
15	H10	0.3973000	0.4803600
butan_2_ol			
1	C1	-0.0892000	-0.0891975
2	C2	-0.1147000	-0.1109575
3	C3	-0.0867000	-0.0829575
4	C4	0.1416000	0.1712000
5	O1	-0.6028000	-0.7288175
6	H1	0.0357000	0.0357000
7	H2	0.0357000	0.0357000
8	H3	0.0357000	0.0357000
9	H4	0.0421000	0.0421000
10	H5	0.0421000	0.0421000
11	H6	0.0421000	0.0421000
12	H7	0.0465000	0.0465000
13	H8	0.0465000	0.0465000
14	H9	0.0268000	0.0324000
15	H10	0.3986000	0.4819300
cycloheptanol			
1	C1	-0.0732000	-0.0731986
2	C2	-0.0732000	-0.0731986
3	C3	-0.0689000	-0.0688986
4	C4	-0.0689000	-0.0688986
5	C5	-0.0974000	-0.0963786
6	C6	-0.0974000	-0.0963786
7	C7	0.1469000	0.1776100
8	O1	-0.6057000	-0.7323186
9	H1	0.0372000	0.0372000
10	H2	0.0372000	0.0372000
11	H3	0.0372000	0.0372000
12	H4	0.0372000	0.0372000
13	H5	0.0387000	0.0387000
14	H6	0.0387000	0.0387000
15	H7	0.0387000	0.0387000
16	H8	0.0387000	0.0387000
17	H9	0.0463000	0.0463000
18	H10	0.0463000	0.0463000
19	H11	0.0463000	0.0463000
20	H12	0.0463000	0.0463000

21	H13	0.0524000	0.0633500
22	H14	0.3966000	0.4795100
cyclohexanol			
1	C1	-0.0753000	-0.0753000
2	C2	-0.0723000	-0.0723000
3	C3	-0.0723000	-0.0723000
4	C4	-0.0907000	-0.0874700
5	C5	-0.0907000	-0.0874700
6	C6	0.1440000	0.1741000
7	O1	-0.6027000	-0.7286900
8	H1	0.0389000	0.0389000
9	H2	0.0389000	0.0389000
10	H3	0.0411000	0.0411000
11	H4	0.0411000	0.0411000
12	H5	0.0411000	0.0411000
13	H6	0.0411000	0.0411000
14	H7	0.0475000	0.0475000
15	H8	0.0475000	0.0475000
16	H9	0.0475000	0.0475000
17	H10	0.0475000	0.0475000
18	H11	0.0297000	0.0359100
19	H12	0.3981000	0.4813200
cyclopentanol			
1	C1	-0.0766000	-0.0766000
2	C2	-0.0766000	-0.0766000
3	C3	-0.0966000	-0.0940500
4	C4	-0.0966000	-0.0940500
5	C5	0.1345000	0.1626200
6	O1	-0.5961000	-0.7207100
7	H1	0.0426000	0.0426000
8	H2	0.0426000	0.0426000
9	H3	0.0426000	0.0426000
10	H4	0.0426000	0.0426000
11	H5	0.0501000	0.0501000
12	H6	0.0501000	0.0501000
13	H7	0.0501000	0.0501000
14	H8	0.0501000	0.0501000
15	H9	0.0381000	0.0460600
16	H10	0.3991000	0.4825300
decan_1_ol			
1	C1	-0.0896000	-0.0896000
2	C2	-0.0777000	-0.0777000
3	C3	-0.0768000	-0.0768000
4	C4	-0.0765000	-0.0765000
5	C5	-0.0761000	-0.0761000
6	C6	-0.0768000	-0.0768000
7	C7	-0.0761000	-0.0761000
8	C8	-0.0759000	-0.0759000
9	C9	-0.0790000	-0.0720000
10	C10	0.1340000	0.1620100
11	O1	-0.6034000	-0.7295400
12	H1	0.0314000	0.0314000
13	H2	0.0314000	0.0314000
14	H3	0.0314000	0.0314000
15	H4	0.0368000	0.0368000
16	H5	0.0368000	0.0368000
17	H6	0.0382000	0.0382000
18	H7	0.0382000	0.0382000
19	H8	0.0383000	0.0383000
20	H9	0.0383000	0.0383000
21	H10	0.0378000	0.0378000
22	H11	0.0378000	0.0378000
23	H12	0.0391000	0.0391000
24	H13	0.0391000	0.0391000
25	H14	0.0383000	0.0383000
26	H15	0.0383000	0.0383000
27	H16	0.0425000	0.0425000
28	H17	0.0425000	0.0425000
29	H18	0.0509000	0.0509000
30	H19	0.0509000	0.0509000
31	H20	0.0187000	0.0226100
32	H21	0.0187000	0.0226100

33	H22	0.3985000	0.4818100
ethanol			
1	C1	-0.1329000	-0.1347150
2	C2	0.1287000	0.1556000
3	O1	-0.6013000	-0.7269950
4	H1	0.0414000	0.0414000
5	H2	0.0414000	0.0414000
6	H3	0.0414000	0.0414000
7	H4	0.0423000	0.0511400
8	H5	0.0423000	0.0511400
9	H6	0.3967000	0.4796300
heptan_1_ol			
1	C1	-0.0898000	-0.0898000
2	C2	-0.0781000	-0.0781000
3	C3	-0.0770000	-0.0770000
4	C4	-0.0767000	-0.0767000
5	C5	-0.0760000	-0.0760000
6	C6	-0.1169000	-0.1194700
7	C7	0.1299000	0.1570600
8	O1	-0.6006000	-0.7261600
9	H1	0.0318000	0.0318000
10	H2	0.0318000	0.0318000
11	H3	0.0318000	0.0318000
12	H4	0.0377000	0.0377000
13	H5	0.0377000	0.0377000
14	H6	0.0387000	0.0387000
15	H7	0.0387000	0.0387000
16	H8	0.0392000	0.0392000
17	H9	0.0392000	0.0392000
18	H10	0.0415000	0.0415000
19	H11	0.0415000	0.0415000
20	H12	0.0463000	0.0463000
21	H13	0.0463000	0.0463000
22	H14	0.0430000	0.0519900
23	H15	0.0430000	0.0519900
24	H16	0.3970000	0.4799900
hexan_1_ol			
1	C1	-0.0899000	-0.0899000
2	C2	-0.0778000	-0.0778000
3	C3	-0.0767000	-0.0767000
4	C4	-0.0744000	-0.0744000
5	C5	-0.1166000	-0.1191700
6	C6	0.1294000	0.1564500
7	O1	-0.6001000	-0.7255500
8	H1	0.0319000	0.0319000
9	H2	0.0319000	0.0319000
10	H3	0.0319000	0.0319000
11	H4	0.0380000	0.0380000
12	H5	0.0380000	0.0380000
13	H6	0.0390000	0.0390000
14	H7	0.0390000	0.0390000
15	H8	0.0421000	0.0421000
16	H9	0.0421000	0.0421000
17	H10	0.0446000	0.0446000
18	H11	0.0446000	0.0446000
19	H12	0.0432000	0.0522300
20	H13	0.0432000	0.0522300
21	H14	0.3966000	0.4795100
hexan_3_ol			
1	C1	-0.0904000	-0.0904000
2	C2	-0.0892000	-0.0892000
3	C3	-0.0777000	-0.0777000
4	C4	-0.0764000	-0.0729400
5	C5	-0.1083000	-0.1048400
6	C6	0.1433000	0.1732600
7	O1	-0.6030000	-0.7290600
8	H1	0.0327000	0.0327000
9	H2	0.0327000	0.0327000
10	H3	0.0327000	0.0327000
11	H4	0.0354000	0.0354000
12	H5	0.0354000	0.0354000
13	H6	0.0354000	0.0354000

14	H7	0.0412000	0.0412000
15	H8	0.0412000	0.0412000
16	H9	0.0478000	0.0478000
17	H10	0.0478000	0.0478000
18	H11	0.0464000	0.0464000
19	H12	0.0464000	0.0464000
20	H13	0.0281000	0.0339700
21	H14	0.3985000	0.4818100
m_cresol			
1	C1	-0.0885000	-0.0884986
2	C2	-0.1665000	-0.1664986
3	C3	-0.2182000	-0.2229286
4	C4	-0.1588000	-0.1635286
5	C5	-0.0334000	-0.0333986
6	C6	0.1270000	0.1535500
7	C7	-0.0633000	-0.0632986
8	O1	-0.5006000	-0.6052486
9	H1	0.1317000	0.1317000
10	H2	0.1330000	0.1330000
11	H3	0.1325000	0.1325000
12	H4	0.1495000	0.1495000
13	H5	0.0456000	0.0456000
14	H6	0.0456000	0.0456000
15	H7	0.0456000	0.0456000
16	H8	0.4188000	0.5063500
methanol			
1	C1	0.1201000	0.1452100
2	O1	-0.6003000	-0.7257900
3	H1	0.0277000	0.0334900
4	H2	0.0277000	0.0334900
5	H3	0.0277000	0.0334900
6	H4	0.3971000	0.4801100
nonan_1_ol			
1	C1	-0.0898000	-0.0898000
2	C2	-0.0781000	-0.0781000
3	C3	-0.0768000	-0.0768000
4	C4	-0.0762000	-0.0762000
5	C5	-0.0762000	-0.0762000
6	C6	-0.0776000	-0.0776000
7	C7	-0.0765000	-0.0765000
8	C8	-0.1168000	-0.1194300
9	C9	0.1300000	0.1571800
10	O1	-0.6008000	-0.7264000
11	H1	0.0316000	0.0316000
12	H2	0.0316000	0.0316000
13	H3	0.0316000	0.0316000
14	H4	0.0375000	0.0375000
15	H5	0.0375000	0.0375000
16	H6	0.0383000	0.0383000
17	H7	0.0383000	0.0383000
18	H8	0.0385000	0.0385000
19	H9	0.0385000	0.0385000
20	H10	0.0386000	0.0386000
21	H11	0.0386000	0.0386000
22	H12	0.0395000	0.0395000
23	H13	0.0395000	0.0395000
24	H14	0.0416000	0.0416000
25	H15	0.0416000	0.0416000
26	H16	0.0463000	0.0463000
27	H17	0.0463000	0.0463000
28	H18	0.0432000	0.0522300
29	H19	0.0432000	0.0522300
30	H20	0.3970000	0.4799900
o_cresol			
1	C1	-0.1608000	-0.1608000
2	C2	-0.0974000	-0.0974000
3	C3	-0.1006000	-0.1006000
4	C4	-0.2094000	-0.2134200
5	C5	-0.0890000	-0.0930200
6	C6	0.1194000	0.1443600
7	C7	-0.0491000	-0.0491000
8	O1	-0.4990000	-0.6033200

9	H1	0.1327000	0.1327000
10	H2	0.1319000	0.1319000
11	H3	0.1339000	0.1339000
12	H4	0.1319000	0.1319000
13	H5	0.0458000	0.0458000
14	H6	0.0458000	0.0458000
15	H7	0.0458000	0.0458000
16	H8	0.4181000	0.5055000
octan_1_ol			
1	C1	-0.0898000	-0.0898000
2	C2	-0.0781000	-0.0781000
3	C3	-0.0772000	-0.0772000
4	C4	-0.0767000	-0.0767000
5	C5	-0.0770000	-0.0770000
6	C6	-0.0758000	-0.0758000
7	C7	-0.1169000	-0.1195300
8	C8	0.1297000	0.1568100
9	O1	-0.6005000	-0.7260300
10	H1	0.0317000	0.0317000
11	H2	0.0317000	0.0317000
12	H3	0.0317000	0.0317000
13	H4	0.0375000	0.0375000
14	H5	0.0375000	0.0375000
15	H6	0.0387000	0.0387000
16	H7	0.0387000	0.0387000
17	H8	0.0387000	0.0387000
18	H9	0.0387000	0.0387000
19	H10	0.0390000	0.0390000
20	H11	0.0390000	0.0390000
21	H12	0.0420000	0.0420000
22	H13	0.0420000	0.0420000
23	H14	0.0460000	0.0460000
24	H15	0.0460000	0.0460000
25	H16	0.0432000	0.0522300
26	H17	0.0432000	0.0522300
27	H18	0.3970000	0.4799900
p_cresol			
1	C1	-0.0949000	-0.0949000
2	C2	-0.0949000	-0.0949000
3	C3	-0.1813000	-0.1852300
4	C4	-0.1813000	-0.1852300
5	C5	-0.1027000	-0.1027000
6	C6	0.1190000	0.1438789
7	C7	-0.0550000	-0.0550000
8	O1	-0.4999000	-0.6044000
9	H1	0.1331000	0.1330989
10	H2	0.1331000	0.1330989
11	H3	0.1409000	0.1408989
12	H4	0.1409000	0.1408989
13	H5	0.0415000	0.0414989
14	H6	0.0415000	0.0414989
15	H7	0.0415000	0.0414989
16	H8	0.4185000	0.5059889
pentan_1_ol			
1	C1	-0.0899000	-0.0899000
2	C2	-0.0779000	-0.0779000
3	C3	-0.0748000	-0.0748000
4	C4	-0.1124000	-0.1140100
5	C5	0.1298000	0.1569300
6	O1	-0.6005000	-0.7260300
7	H1	0.0321000	0.0321000
8	H2	0.0321000	0.0321000
9	H3	0.0321000	0.0321000
10	H4	0.0380000	0.0380000
11	H5	0.0380000	0.0380000
12	H6	0.0427000	0.0427000
13	H7	0.0427000	0.0427000
14	H8	0.0448000	0.0448000
15	H9	0.0448000	0.0448000
16	H10	0.0408000	0.0493300
17	H11	0.0408000	0.0493300
18	H12	0.3968000	0.4797500

pentan_2_ol			
1	C1	-0.0904000	-0.0903999
2	C2	-0.1245000	-0.1208899
3	C3	-0.0745000	-0.0744999
4	C4	-0.0769000	-0.0732899
5	C5	0.1433000	0.1732592
6	O1	-0.6035000	-0.7296599
7	H1	0.0325000	0.0324992
8	H2	0.0325000	0.0324992
9	H3	0.0325000	0.0324992
10	H4	0.0419000	0.0418992
11	H5	0.0419000	0.0418992
12	H6	0.0419000	0.0418992
13	H7	0.0408000	0.0407992
14	H8	0.0408000	0.0407992
15	H9	0.0480000	0.0479992
16	H10	0.0480000	0.0479992
17	H11	0.0277000	0.0334892
18	H12	0.3980000	0.4811992
pentan_3_ol			
1	C1	-0.0899000	-0.0898999
2	C2	-0.0899000	-0.0898999
3	C3	-0.1087000	-0.1092399
4	C4	-0.1087000	-0.1092399
5	C5	0.1391000	0.1681792
6	O1	-0.5992000	-0.7244599
7	H1	0.0354000	0.0353992
8	H2	0.0354000	0.0353992
9	H3	0.0354000	0.0353992
10	H4	0.0354000	0.0353992
11	H5	0.0354000	0.0353992
12	H6	0.0354000	0.0353992
13	H7	0.0449000	0.0448992
14	H8	0.0449000	0.0448992
15	H9	0.0449000	0.0448992
16	H10	0.0449000	0.0448992
17	H11	0.0688000	0.0831792
18	H12	0.3965000	0.4793892
phenol			
1	C1	-0.1656000	-0.1656000
2	C2	-0.0943000	-0.0943000
3	C3	-0.0943000	-0.0943000
4	C4	-0.1850000	-0.1894600
5	C5	-0.1850000	-0.1894600
6	C6	0.1235000	0.1493186
7	O1	-0.4998000	-0.6042800
8	H1	0.1333000	0.1332986
9	H2	0.1330000	0.1329986
10	H3	0.1330000	0.1329986
11	H4	0.1411000	0.1410986
12	H5	0.1411000	0.1410986
13	H6	0.4190000	0.5065886
prop_2_en_1_ol			
1	C1	-0.2070000	-0.2070000
2	C2	-0.1987000	-0.2084800
3	C3	0.1613000	0.1950200
4	O1	-0.5969000	-0.7216800
5	H1	0.1142000	0.1142000
6	H2	0.1142000	0.1142000
7	H3	0.1305000	0.1305000
8	H4	0.0414000	0.0500500
9	H5	0.0414000	0.0500500
10	H6	0.3996000	0.4831400
propan_1_ol			
1	C1	-0.0888000	-0.0887967
2	C2	-0.1040000	-0.1031367
3	C3	0.1306000	0.1579000
4	O1	-0.6015000	-0.7272367
5	H1	0.0361000	0.0361000
6	H2	0.0361000	0.0361000
7	H3	0.0361000	0.0361000
8	H4	0.0443000	0.0443000

9	H5	0.0443000	0.0443000
10	H6	0.0348000	0.0420700
11	H7	0.0348000	0.0420700
12	H8	0.3972000	0.4802300
propan_2_ol			
1	C1	-0.1270000	-0.1277700
2	C2	-0.1270000	-0.1277700
3	C3	0.1380000	0.1668489
4	O1	-0.6035000	-0.7296600
5	H1	0.0411000	0.0410989
6	H2	0.0411000	0.0410989
7	H3	0.0411000	0.0410989
8	H4	0.0411000	0.0410989
9	H5	0.0411000	0.0410989
10	H6	0.0411000	0.0410989
11	H7	0.0766000	0.0926089
12	H8	0.3963000	0.4791489

## The 'hydroxynator.pl' perl conversion script for hydroxyl moiety modification.

```
#!/usr/bin/perl -w

# program that scales the interactions in a gromacs topology
# written by Chris Fennell

# 03/24/14: minor update to clarify topology section processing

$sigmaScale = 3.21990e-01;
$epsilonScale = 8.45476e-01;
$chargeScale = 1.20905;
$hydroxyl_o = 'oh';
$hydroxyl_h = 'ho';
$tol_bond_h = 0.12;
$charge_tol = 0.00001;

use Getopt::Std;

# get our options
getopts('he:q:s:');

# if we don't have a filename, drop to -h
$opt_h = 'true' if $#ARGV != 0;

# our option output
if ($opt_h){
    print "\n$0: converts sigma, epsilon, or charge OH values in a gromacs topology to
dielectric corrected values\n\n";
    print "usage: $0 [-options] [topology file name] \n\n";
    print "  -h : show this message\n\n";
    print "  -e real : OH epsilon conversion value\n";
    print "              (default: $epsilonScale)\n";
    print "  -q real : OH environment charge scaling fraction\n";
    print "              (default: $chargeScale)\n";
    print "  -s real : OH sigma conversion value\n";
    print "              (default: $sigmaScale)\n\n";
}

# set some variables to be used in the code
$topFileName = $ARGV[0];

if (defined($opt_e)){
    if ($opt_e =~ /^[0-9]/) {
        if ($opt_e < 0){
            die "\t-e value ($opt_e) is not a valid number\n\tPlease choose a real
number greater than 0\n";
        } else {
            $epsilonScale = $opt_e;
        }
    } else {
        die "\t-e value ($opt_e) is not a valid number\n\tPlease choose a real number
greater than 0\n";
    }
}

if (defined($opt_q)){
    if ($opt_q =~ /^[0-9]/) {
        $chargeScale = $opt_q;
    } else {
        die "\t-q value ($opt_q) is not a valid number\n\tPlease choose a real number\n";
    }
}

if (defined($opt_s)){
    if ($opt_s =~ /^[0-9]/) {
        if ($opt_s < 0){
            die "\t-s value ($opt_s) is not a valid number\n\tPlease choose a real
number greater than 0\n";
        } else {
            $sigmaScale = $opt_s;
        }
    } else {

```

```

        die "\t-s value ($opt_s) is not a valid number\n\tPlease choose a real number
greater than 0\n";
    }
}

# some input checking

open(STATFILE, ".$stopFileName") || die "\tError: can't find file $stopFileName\n";

$types_sec = 0;
$atoms_sec = 0;
$bonds_sec = 0;
$stop_output = 0;

while (<STATFILE>){ @line = split;
    if (defined($line[1]) && $line[1] eq 'atomtypes'){
        $types_sec = 1;
    } if (defined($line[1]) && $line[1] eq 'atoms'){
        $atoms_sec = 1;
        $stop_output = 1;
    } if (defined($line[1]) && $line[1] eq 'bonds'){
        $bonds_sec = 1;
        $atoms_sec = 0;
    } if (defined($line[1]) && $line[1] eq 'pairs'){
        $bonds_sec = 0;
        $atoms_sec = 0;
    } if (defined($line[1]) && $line[1] eq 'moleculetype'){
        $types_sec = 0;
    } if (defined($line[1]) && $line[1] eq 'constraints'){
        $atoms_sec = 0;
        $bonds_sec = 0;
    }
}

if (defined($line[0])){
    $first_char = substr($line[0], 0, 1);
    if ($types_sec == 1 && $first_char ne ';'){
        if ($sigmaScale != 1 || $epsilonScale != 1){
            if ($#line >= 6){
                if ($line[0] eq $hydroxyl_o){
                    $line[5] = $sigmaScale;
                    $line[6] = $epsilonScale;
                    printf("%-5s%11s%12.4f%8.4f%3s%14.5e%13.5e\n", $line[0], $line[1], $line[2],
$line[3], $line[4], $line[5], $line[6]);
                } else {
                    printf("%-5s%11s%12.4f%8.4f%3s%14.5e%13.5e\n", $line[0], $line[1], $line[2],
$line[3], $line[4], $line[5], $line[6]);
                }
            } else {
                print $_;
            }
        } else {
            print $_;
        }
    } elseif ($atoms_sec == 1 && $first_char ne ';' && $first_char ne '['){
# Save the atoms sections for processing
        push(@atoms_lines0, $line[0]);
        push(@atoms_lines1, $line[1]);
        push(@atoms_lines2, $line[2]);
        push(@atoms_lines3, $line[3]);
        push(@atoms_lines4, $line[4]);
        push(@atoms_lines5, $line[5]);
        push(@atoms_lines6, $line[6]);
        push(@atoms_lines7, $line[7]);
    } elseif ($bonds_sec == 1 && $first_char ne ';' && $first_char ne '['){
# Save the bond connections for processing
        push(@bond_i, $line[0]);
        push(@bond_j, $line[1]);
        push(@bond_lengths, $line[3]);
    } elseif ($stop_output == 0) {
        print $_;
    }
} elseif ($stop_output == 0) {

```

```

    print $_;
  }
}

close(STATFILE);

# Identify hydroxyl O and H atoms
for ($i = 0; $i<=$#atoms_lines0; $i++){
  if ($atoms_lines1[$i] eq $hydroxyl_o){
    push(@hydroxyl_o_numbers, $atoms_lines0[$i]);
    push(@full_scale, $atoms_lines0[$i]);
  } elsif ($atoms_lines1[$i] eq $hydroxyl_h){
    push(@hydroxyl_h_numbers, $atoms_lines0[$i]);
    push(@full_scale, $atoms_lines0[$i]);
  }
}

$hydroxyl_count = $#hydroxyl_o_numbers + 1;
print STDERR "\n$hydroxyl_count hydroxyl moieties identified...\n\n";

# Now identify hydroxyl bonded carbon atoms
for ($i = 0; $i<=$#hydroxyl_o_numbers; $i++){
  $current_o = $hydroxyl_o_numbers[$i];
  for ($j = 0; $j<=$#bond_i; $j++){
    if ($bond_i[$j] == $current_o){
      $is_hydrogen = 0;
      for ($k = 0; $k<=$#hydroxyl_h_numbers; $k++){
        if ($bond_j[$j] == $hydroxyl_h_numbers[$k]){
          $is_hydrogen = 1;
        }
      }
      if ($is_hydrogen == 0){
        push(@other_bonded, $bond_j[$j]);
      }
    }
  }
}

# and loop over bond_j vals
if ($bond_j[$j] == $current_o){
  $is_hydrogen = 0;
  for ($k = 0; $k<=$#hydroxyl_h_numbers; $k++){
    if ($bond_i[$j] == $hydroxyl_h_numbers[$k]){
      $is_hydrogen = 1;
    }
  }
  if ($is_hydrogen == 0){
    push(@other_bonded, $bond_i[$j]);
  }
}
}

# fill the full charge scaling array
for ($i=0; $i<=$#other_bonded; $i++){
  push(@full_scale, $other_bonded[$i]);
}

# loop over the other_bondeds to identify hydrogens
for ($i=0; $i<=$#other_bonded; $i++){
  for ($j = 0; $j<=$#bond_i; $j++){
    if ($bond_i[$j] == $other_bonded[$i]){
      if ($bond_lengths[$j] < $tol_bond_h){
        push(@full_scale, $bond_j[$j]);
      } else {
        $is_oxygen = 0;
        for ($k=0; $k<=$#hydroxyl_o_numbers; $k++){
          if ($bond_j[$j] == $hydroxyl_o_numbers[$k]){
            $is_oxygen = 1;
          }
        }
        push(@neutralize_atoms, $bond_j[$j]) if $is_oxygen == 0;
      }
    }
  }
  if ($bond_j[$j] == $other_bonded[$i]){

```

```

        if ($bond_lengths[$j] < $tol_bond_h){
            push(@full_scale, $bond_i[$j]);
        } else {
            $is_oxygen = 0;
            for ($k=0; $k<=$#hydroxyl_o_numbers; $k++){
                if ($bond_i[$j] == $hydroxyl_o_numbers[$k]){
                    $is_oxygen = 1;
                }
            }
            push(@neutralize_atoms, $bond_i[$j]) if $is_oxygen == 0;
        }
    }
}

# sort our arrays
@full_scale = sort(@full_scale);
@neutralize_atoms = sort(@neutralize_atoms);

# scan for conflicts in the full_scale and neutralize_atoms lists
if ($#full_scale >= $#neutralize_atoms){
    for ($i=0; $i<=$#full_scale; $i++){
        for ($j=0; $j<=$#neutralize_atoms; $j++){
            if ($full_scale[$i] == $neutralize_atoms[$j]){
                push(@dont_neutralize, $neutralize_atoms[$j]);
            }
        }
    }
}

for ($i=0; $i<=$#dont_neutralize; $i++){
    print STDERR "Warning: atom $dont_neutralize[$i] is at a junction between hydroxyl charge
scaling groups.\n\tThis atom will be fully scaled rather than used as a neutralization site.\n";
}

# make a new neutralization list
if ($#dont_neutralize >= 0){
    for ($i=0; $i<=$#neutralize_atoms; $i++){
        $is_present = 0;
        for ($j=0; $j<=$#dont_neutralize; $j++){
            if ($neutralize_atoms[$i] == $dont_neutralize[$j]){
                $is_present = 1;
            }
        }
        push(@temp_neutralize_atoms, $neutralize_atoms[$i]) if $is_present == 0;
    }
    $#neutralize_atoms = -1;
    @neutralize_atoms = @temp_neutralize_atoms;
}
@neutralize_atoms = sort(@neutralize_atoms);

# okay, let's scale charges
$old_charge = 0;
$new_charge = 0;

for ($i=0; $i<=$#full_scale; $i++){
    $index_val = $full_scale[$i] - 1;
    $old_charge += $atoms_lines6[$index_val];
    $atoms_lines6[$index_val] *= $chargeScale;
    $new_charge += $atoms_lines6[$index_val];
}

# now, let's distribute the remaining charge difference to the neutralization atoms
$charge_diff = $new_charge - $old_charge;
if ($#neutralize_atoms >= 0){
    $charge_diff /= ($#neutralize_atoms + 1);

    for ($i=0; $i<=$#neutralize_atoms; $i++){
        $index_val = $neutralize_atoms[$i] - 1;
        $atoms_lines6[$index_val] -= $charge_diff;
    }
} else {

```

```

# if there are no neutralization atoms, subtract charge equally from all
$charge_diff /= ($#atoms_lines6 + 1);
for ($i=0; $i<=$#atoms_lines6; $i++){
    $atoms_lines6[$i] -= $charge_diff;
}
}

# make sure the molecule is neutral... warn if not
$total_charge = 0;
for ($i=0; $i<=$#atoms_lines6; $i++){
    $atoms_lines6[$i] = sprintf("%11.6f", $atoms_lines6[$i]);
    $total_charge += $atoms_lines6[$i];
}
if (abs($total_charge) >= $charge_tol){
    print STDERR "Warning: After scaling, the molecule had a net charge of $total_charge\n\tIf you
want a neutral molecule, redistribute this charge manually";
}

# now we reprocess the STATFILE to finish out output scaling
open(STATFILE, ".$topFileName") || die "\tError: can't find file $topFileName\n";
$start_output = 0;

while (<STATFILE>){
    @line = split;

    if (defined($line[1]) && $line[1] eq 'atomtypes'){
        $types_sec = 1;
    } if (defined($line[1]) && $line[1] eq 'atoms'){
        $atoms_sec = 1;
        $start_output = 1;
        $output_count = 0;
    } if (defined($line[1]) && $line[1] eq 'moleculetype'){
        $types_sec = 0;
    } if (defined($line[1]) && $line[1] eq 'bonds'){
        $atoms_sec = 0;
    } if (defined($line[1]) && $line[1] eq 'constraints'){
        $atoms_sec = 0;
    }

    if ($start_output == 1){
        if (defined($line[0])){
            $first_char = substr($line[0], 0, 1);
            if ($atoms_sec == 1 && $first_char ne ';' && $first_char ne '['){
                printf("%6d%11s%7d%8s%6s%7d%11.5f%11.6f\n",
                    $atoms_lines0[$output_count],
                    $atoms_lines1[$output_count],
                    $atoms_lines2[$output_count],
                    $atoms_lines3[$output_count],
                    $atoms_lines4[$output_count],
                    $atoms_lines5[$output_count],
                    $atoms_lines6[$output_count],
                    $atoms_lines7[$output_count]);
                $output_count++;
            } else {
                print $_;
            }
        } else {
            print $_;
        }
    }
}
}

```

## The 'hydroxynator.py' python conversion script for hydroxyl moiety modification.

```
#!/bin/env python

import os
from math import *

"""Implements the new GAFF hydroxyl parameterization of Fennell, Wymer, and Mobley (2014), which
involves scaling partial charges on hydroxyl and some surrounding atoms, and new LJ parameters
for hydroxyl oxygens.

Written by David Mobley, modeled after hydroxynator.pl by Chris Fennell. This means the current
implementation is relatively un-Pythonic, but it works.

Change Log:
- First version, 11/20/13
- 11/21/13: Fixed bug with tolerance for hydrogen bond lengths; fixed output file name; added
option for output topology file name to have different name from input topology file.
"""

sigmaScale = 3.21990e-01
epsilonScale = 8.45476e-01
chargeScale = 1.20905
hydroxyl_o = 'oh'
hydroxyl_h = 'ho'
tol_bond_h = 0.12
charge_tol = 0.00001

#Configure input options
from optparse import OptionParser
parser = OptionParser(usage = "Converts sigma, epsilon, and charge OH values in a GROMACS
topology to dielectric corrected values.\nUsage: [-options] [topology file name] \n\n", epilog =
"Note: Assumes hydroxyl oxygens and hydrogens follow standard GAFF naming ('%s' and '%s'
respectively; if you have hydroxyls with other atom names you will need to adjust the source
code.)" % (hydroxyl_o, hydroxyl_h))
#Check on -h
parser.add_option('-e', help='OH epsilon conversion value, if other than standard. Default: %.5g'
% epsilonScale, default = epsilonScale, type = "float", dest = 'epsilonScale')
parser.add_option('-q', help='OH environment charge scaling fraction, if other than standard.
Default: %.5f' % chargeScale, default = chargeScale, type = "float", dest = 'chargeScale')
parser.add_option('-s', help='OH sigma conversion value, if other than standard. Default: %.5g' %
sigmaScale, default = sigmaScale, type = "float", dest = 'sigmaScale')
parser.add_option('-o', help='Output topology file name. Default: Edit input topology file. If
specified, instead creates new output topology file.', dest = 'outtop', type = "string" )

(options, args) = parser.parse_args()
epsilonScale = options.epsilonScale
sigmaScale = options.sigmaScale
chargeScale = options.chargeScale
topfile = args[0]
if not options.outtop:
    outtop = topfile
else:
    outtop = options.outtop

if not os.path.isfile( topfile):
    parser.error('"%s" is not a topology file I can find. Please enter the name of a valid
topology file.' % topfile )

#Now process, basically following Fennell algorithm from hydroxynator.pl
file = open(topfile, 'r')
text = file.readlines()
file.close()
types_sec = False
atoms_sec = False
bonds_sec = False
stop_output = False
outtext = []
atom_columns = {}
```

```

bond_i = []
bond_j = []
bond_lengths = []
for line in text:
    if line[0]!=';': #Skip lines beginning with comments
        outtext.append(line)
        continue
    if '[ atomtypes ]' in line or '[atomtypes]' in line:
        types_sec = True
    elif '[ atoms ]' in line or '[atoms]' in line:
        atoms_sec = True
        stop_output = True
    elif '[ bonds ]' in line or '[bonds]' in line:
        bonds_sec = True
        atoms_sec = False
    elif '[ pairs ]' in line or '[pairs]' in line:
        bonds_sec = False
    elif '[ moleculetype ]' in line or '[moleculetype]' in line:
        types_sec = False
    elif '[ constraints ]' in line or '[constraints]' in line:
        bonds_sec = True
    #Why is constraints treated like a bonds section?
        atoms_sec = False

    tmp = line.split()
    if len(tmp)>1 and tmp[0][0] <> ';' and tmp[0][0] <> '[':
        if types_sec and sigmaScale <> 1. and epsilonScale <> 1.: #If we're scaling LJ and we're
in the atom types section
            if len(tmp) >= 6: #Update values
                if tmp[0] == hydroxyl_o: #If we have a hydroxyl oxygen
                    tmp[5] = sigmaScale
                    tmp[6] = epsilonScale
                    #Re-build line
                    line = "%-5s%11s%12.4f%8.4f%3s%14.5e%13.5e\n" % (tmp[0], tmp[1], float(tmp[2]),
float(tmp[3]), tmp[4], float(tmp[5]), float(tmp[6]))
                elif atoms_sec:
                    #Save the atoms section for processing
                    tmp = line.split()
                    for (idx, elem) in enumerate(tmp):
                        if not atom_columns.has_key(idx): atom_columns[idx] = []
                        if idx==6: #If the charge, go ahead and make it a float
                            atom_columns[idx].append( float(elem) )
                        else:
                            atom_columns[idx].append( elem )
                elif bonds_sec:
                    bond_i.append( tmp[0] )
                    bond_j.append( tmp[1] )
                    bond_lengths.append( float(tmp[3]) )
                #elif not stop_output:
                #    outtext.append(line)
            #elif not stop_output:
            #    outtext.append(line)
        outtext.append(line)

#Find hydroxyl O and H atoms, track their atom numbers
n_atom_lines = len(atom_columns[0] ) #Number of atom lines
full_scale = [] #Atoms with charges which will be fully scaled
hydroxyl_o_numbers = [] #Hydroxyl oxgen indices
hydroxyl_h_numbers = []
for n in range(n_atom_lines):
    atrn = atom_columns[0][n]
    if atom_columns[1][n] == hydroxyl_o:
        full_scale.append( atrn )
        hydroxyl_o_numbers.append( atrn )
    elif atom_columns[1][n] == hydroxyl_h:
        hydroxyl_h_numbers.append( atrn )
        full_scale.append( atrn )

hydroxyl_count = len(hydroxyl_o_numbers)
print "\n%s hydroxyl moieties identified...\n\n" % hydroxyl_count

```

```

if not len(hydroxyl_h_numbers) == len(hydroxyl_o_numbers):
    print "WARNING: Unequal numbers of hydroxyl oxygens and hydrogens found."

#Now identify hydroxyl bonded carbon atoms
other_bonded = []
for i in range(hydroxyl_count): #Loop over all oxygens
    current_o = hydroxyl_o_numbers[i]
    for j in range( len(bond_i) ): #Find bond involving this oxygen
        if bond_i[j] == current_o:
            is_hydrogen = False
            if bond_j[j] in hydroxyl_h_numbers:
                is_hydrogen = True
            if not is_hydrogen:
                other_bonded.append( bond_j[j] )
    #Similarly check bond_j to see if one of them is this oxygen
    if bond_j[j] == current_o:
        is_hydrogen = False
        if bond_i[j] in hydroxyl_h_numbers:
            is_hydrogen = True
        if not is_hydrogen:
            other_bonded.append(bond_i[j] )

#Fill in the full charge scaling array
neutralize_atoms = []
for i in range(len(other_bonded)):
    full_scale.append(other_bonded[i])

#Loop over the other bondeds to identify hydrogens
for i in range(len(other_bonded)):
    for j in range(len(bond_i)):
        if bond_i[j] == other_bonded[i]:
            if bond_lengths[j] < tol_bond_h:
                full_scale.append( bond_j[j] )
            else:
                is_oxygen = False
                if bond_j[j] in hydroxyl_o_numbers:
                    is_oxygen = True
                if not is_oxygen:
                    neutralize_atoms.append( bond_j[j] )
        if bond_j[j] == other_bonded[i]:
            if bond_lengths[j] < tol_bond_h:
                full_scale.append( bond_i[j] )
            else:
                is_oxygen = False
                if bond_i[j] in hydroxyl_o_numbers:
                    is_oxygen = True
                if not is_oxygen:
                    neutralize_atoms.append( bond_i[j] )

#Sort arrays
full_scale.sort()
neutralize_atoms.sort()

#Scan for conflicts in the full_scale and neutralize_atoms lists
dont_neutralize = []
if len(full_scale) >= len(neutralize_atoms):
    for i in range(len(full_scale)):
        if full_scale[i] in neutralize_atoms:
            dont_neutralize.append( full_scale[i] )

for i in range(len(dont_neutralize)):
    print "WARNING: atom %s is at a junction between hydroxyl charge scaling groups.\n\t This
atom will be fully scaled rather than used as a neutralization site.\n" % dont_neutralize[i]

#Make a new neutralization list which removes these atoms from the neutralization list
if len(dont_neutralize) > 0:
    neutralize_atoms = [ n for n in neutralize_atoms if not n in dont_neutralize ]

neutralize_atoms.sort()

#Scale charges

```

```

old_charge = 0.;
new_charge = 0.;
for i in range(len(full_scale)):
    n = int(full_scale[i])-1
    old_charge += atom_columns[6][n]
    atom_columns[6][n] *= chargeScale
    new_charge += atom_columns[6][n]

#Distribute remaining charge to neutralization atoms
charge_diff = new_charge - old_charge
if len(neutralize_atoms)>0:
    charge_diff /= float(len(neutralize_atoms))

    for i in range(len(neutralize_atoms)):
        n = int(neutralize_atoms[i])-1
        atom_columns[6][n] -= charge_diff
else: #If no neutralization atoms, subtract charge equally from all
    charge_diff /= float(len(atom_columns[6]))
    for i in range(len(atom_columns[6])):
        atom_columns[6][i] -= charge_diff

#Now check if the molecule is neutral and warn if not
total_charge = 0.
for i in range(len(atom_columns[6])):
    total_charge += atom_columns[6][i]

if abs(total_charge) >= charge_tol:
    print "WARNING: After scaling, the molecule had a net charge of %s.\n\t If you want a neutral
molecule, redistribute this charge manually." % total_charge

#Now modify the atoms section in our stored topology file
#Find where atoms section starts
idx = 0
line = outtext[idx]
while '[ atoms ]' not in line and '[atoms]' not in line:
    idx+=1
    line = outtext[idx]
atomstart = idx+1
#Find where atoms section ends
line = outtext[idx]
while '[ bonds ]' not in line and '[bonds]' not in line:
    idx+=1
    line = outtext[idx]
atomend = idx

outct = 0
for idx in range(atomstart, atomend):
    tmp = outtext[idx].split()
    if len(tmp)>1:
        if not ';' in tmp[0] and not '[' in tmp[0]:
            outtext[idx] = "%6d%11s%7d%8s%6s%7d%11.7f%11.6f\n" % ( int(atom_columns[0][outct]),
atom_columns[1][outct], int(atom_columns[2][outct]), atom_columns[3][outct], atom_columns[4]
[outct], int(atom_columns[5][outct]), round(atom_columns[6][outct],7), float(atom_columns[7]
[outct]) )
            outct+=1

file = open(outtop, 'w')
file.writelines(outtext)
file.close()

```